



Full wwPDB X-ray Structure Validation Report ⓘ

Sep 4, 2019 – 12:53 PM EDT

PDB ID : 6RD3
Title : Crystal structure of the wild type OmpK36 from Klebsiella pneumonia
Authors : Beis, K.; Romano, M.; Kwong, J.
Deposited on : 2019-04-12
Resolution : 1.98 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

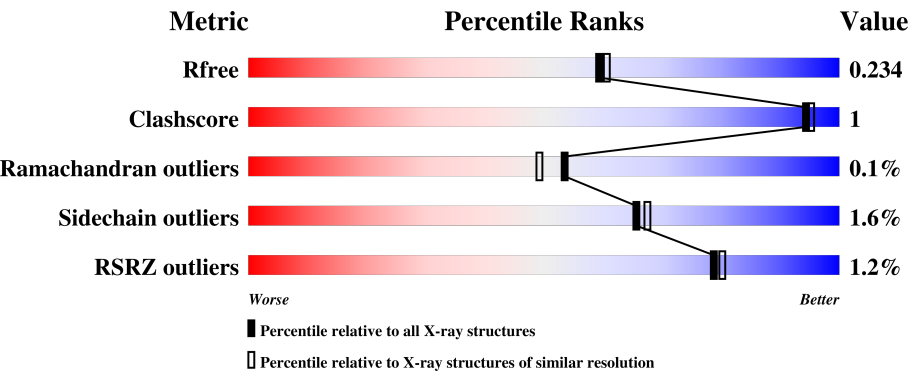
MolProbity : 4.02b-467
Mogul : 1.8.0 (224370), CSD as540be (2019)
Xtriage (Phenix) : 1.13
EDS : 2.4
buster-report : 1.1.7 (2018)
Percentile statistics : 20171227.v01 (using entries in the PDB archive December 27th 2017)
Refmac : 5.8.0158
CCP4 : 7.0 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.4

1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 1.98 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R _{free}	111664	10189 (2.00-1.96)
Clashscore	122126	11405 (2.00-1.96)
Ramachandran outliers	120053	11281 (2.00-1.96)
Sidechain outliers	120020	11280 (2.00-1.96)
RSRZ outliers	108989	9953 (2.00-1.96)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	345	<div><div>2%</div><div>96%</div><div>..</div></div>
1	B	345	<div><div>2%</div><div>93%</div><div>7%</div></div>
1	C	345	<div><div>2%</div><div>96%</div><div>..</div></div>
1	D	345	<div><div>2%</div><div>95%</div><div>5%</div></div>
1	E	345	<div><div>2%</div><div>94%</div><div>6%</div></div>

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Mol	Chain	Length	Quality of chain
1	F	345	<div><div></div><div>2%</div><div>97%</div><div></div></div>

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 17283 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

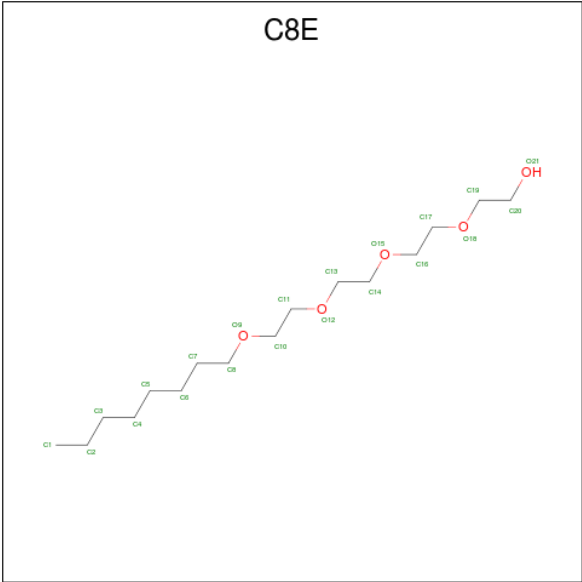
- Molecule 1 is a protein called OmpK36.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	342	Total	C	N	O	S	0	0	0
			2669	1671	448	548	2			
1	B	345	Total	C	N	O	S	0	0	0
			2695	1688	452	553	2			
1	C	342	Total	C	N	O	S	0	0	0
			2665	1667	448	548	2			
1	D	345	Total	C	N	O	S	0	0	0
			2695	1688	452	553	2			
1	E	345	Total	C	N	O	S	0	0	0
			2695	1688	452	553	2			
1	F	345	Total	C	N	O	S	0	0	0
			2695	1688	452	553	2			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	0	GLY	-	expression tag	UNP D6QLY0
B	0	GLY	-	expression tag	UNP D6QLY0
C	0	GLY	-	expression tag	UNP D6QLY0
D	0	GLY	-	expression tag	UNP D6QLY0
E	0	GLY	-	expression tag	UNP D6QLY0
F	0	GLY	-	expression tag	UNP D6QLY0

- Molecule 2 is (HYDROXYETHYLOXY)TRI(ETHYLOXY)OCTANE (three-letter code: C8E) (formula: C₁₆H₃₄O₅).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			9	8	1		
2	A	1	Total	C	O	0	0
			9	8	1		
2	A	1	Total	C	O	0	0
			14	9	5		
2	A	1	Total	C	O	0	0
			11	7	4		
2	A	1	Total	C	O	0	0
			10	6	4		
2	A	1	Total	C	O	0	0
			11	10	1		
2	A	1	Total	C	O	0	0
			12	8	4		
2	B	1	Total	C	O	0	0
			8	7	1		
2	B	1	Total	C		0	0
			7	7			
2	B	1	Total	C	O	0	0
			9	8	1		
2	B	1	Total	C	O	0	0
			9	8	1		
2	B	1	Total	C		0	0
			8	8			
2	B	1	Total	C	O	0	0
			10	9	1		
2	B	1	Total	C	O	0	0
			12	8	4		

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	B	1	Total C O 10 9 1	0	0
2	C	1	Total C O 9 6 3	0	0
2	C	1	Total C O 7 4 3	0	0
2	D	1	Total C O 7 5 2	0	0
2	D	1	Total C O 12 10 2	0	0
2	D	1	Total C O 9 8 1	0	0
2	D	1	Total C O 12 8 4	0	0
2	E	1	Total C O 9 8 1	0	0
2	E	1	Total C 7 7	0	0
2	E	1	Total C O 12 10 2	0	0
2	E	1	Total C O 10 6 4	0	0
2	E	1	Total C 6 6	0	0
2	F	1	Total C 8 8	0	0
2	F	1	Total C O 8 5 3	0	0
2	F	1	Total C O 16 11 5	0	0

- Molecule 3 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	D	1	Total Mg 1 1	0	0
3	E	1	Total Mg 1 1	0	0
3	B	1	Total Mg 1 1	0	0
3	C	1	Total Mg 1 1	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total 1	Mg 1	0	0
3	F	1	Total 1	Mg 1	0	0

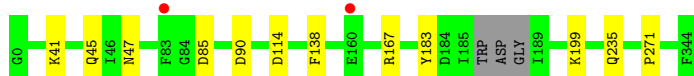
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	156	Total 156	O 156	0	0
4	B	158	Total 158	O 158	0	0
4	C	137	Total 137	O 137	0	0
4	D	162	Total 162	O 162	0	0
4	E	135	Total 135	O 135	0	0
4	F	134	Total 134	O 134	0	0

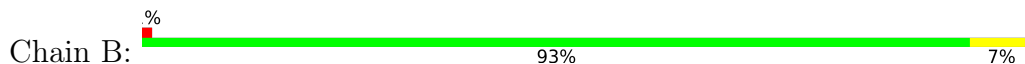
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

- Molecule 1: OmpK36



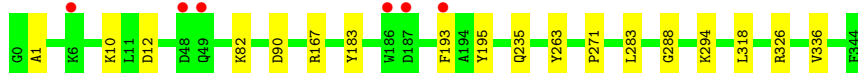
- Molecule 1: OmpK36



- Molecule 1: OmpK36



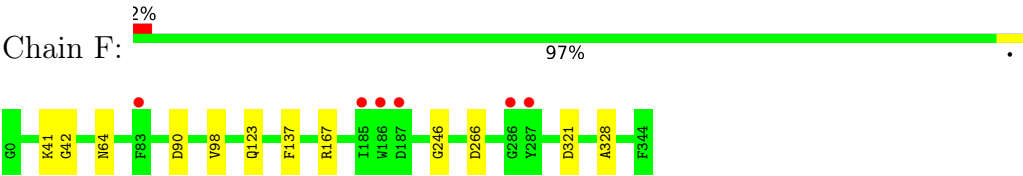
- Molecule 1: OmpK36



- Molecule 1: OmpK36



- Molecule 1: OmpK36



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	55.09Å 316.09Å 73.79Å 90.00° 102.86° 90.00°	Depositor
Resolution (Å)	53.20 – 1.98 53.20 – 1.98	Depositor EDS
% Data completeness (in resolution range)	100.0 (53.20-1.98) 100.0 (53.20-1.98)	Depositor EDS
R_{merge}	0.02	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.49 (at 1.98Å)	Xtriage
Refinement program	PHENIX (1.14_3260: ???)	Depositor
R, R_{free}	0.194 , 0.234 0.194 , 0.234	Depositor DCC
R_{free} test set	8541 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å ²)	22.0	Xtriage
Anisotropy	0.402	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.44 , 61.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	17283	wwPDB-VP
Average B, all atoms (Å ²)	24.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.42% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: MG, C8E

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.39	0/2726	0.57	0/3688
1	B	0.38	0/2755	0.58	0/3730
1	C	0.40	0/2722	0.57	0/3682
1	D	0.39	0/2755	0.58	0/3730
1	E	0.38	0/2755	0.56	0/3730
1	F	0.38	0/2755	0.57	0/3730
All	All	0.39	0/16468	0.57	0/22290

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2669	0	2459	6	0
1	B	2695	0	2477	12	0
1	C	2665	0	2451	3	0
1	D	2695	0	2477	7	0
1	E	2695	0	2477	11	0
1	F	2695	0	2477	4	0
2	A	76	0	111	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	73	0	121	1	0
2	C	16	0	20	0	0
2	D	40	0	61	3	0
2	E	44	0	72	2	0
2	F	32	0	45	0	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
3	E	1	0	0	0	0
3	F	1	0	0	0	0
4	A	156	0	0	0	0
4	B	158	0	0	0	0
4	C	137	0	0	0	0
4	D	162	0	0	0	0
4	E	135	0	0	0	0
4	F	134	0	0	0	0
All	All	17283	0	15248	45	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 1.

All (45) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:48:ASP:HB3	1:B:49:GLN:HE21	1.50	0.76
1:E:26:ASP:HB3	1:E:29:VAL:HG22	1.86	0.57
1:D:294:LYS:HG2	1:D:318:LEU:HB2	1.87	0.56
1:D:193:PHE:HB3	2:D:405:C8E:H202	1.88	0.56
1:E:148:LEU:HD23	1:E:179:THR:HG22	1.89	0.55
1:B:45:GLN:NE2	1:B:47:ASN:O	2.38	0.53
1:D:195:TYR:HB2	2:D:405:C8E:H192	1.91	0.53
1:B:296:VAL:HG11	2:B:801:C8E:H52	1.90	0.52
1:A:45:GLN:NE2	1:A:47:ASN:O	2.33	0.51
1:E:177:PHE:HD2	2:E:404:C8E:H162	1.76	0.51
1:C:4:TYR:HB3	1:C:11:LEU:HB2	1.93	0.49
1:D:1:ALA:N	1:D:12:ASP:OD1	2.46	0.49
1:C:36:MET:HG3	1:C:60:VAL:HB	1.95	0.48
1:A:271:PRO:HB2	2:A:506:C8E:H102	1.95	0.47
1:A:41:LYS:HE2	1:A:41:LYS:HB3	1.59	0.47
1:C:2:GLU:OE1	1:C:10:LYS:HD3	2.13	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:240:TYR:CD2	1:B:253:LYS:HG2	2.50	0.47
1:F:41:LYS:HD2	1:F:42:GLY:N	2.31	0.46
1:E:144:LEU:HD11	1:E:181:LEU:HD11	1.98	0.46
2:A:503:C8E:H191	2:A:503:C8E:H161	1.58	0.45
1:F:266:ASP:N	1:F:266:ASP:OD1	2.49	0.44
1:D:263:TYR:O	1:D:271:PRO:HD2	2.17	0.44
1:B:168:GLY:O	1:B:172:GLN:HG3	2.17	0.44
2:A:505:C8E:H141	2:A:505:C8E:H171	1.69	0.43
1:E:10:LYS:HE3	1:E:10:LYS:HB3	1.72	0.43
1:A:85:ASP:O	1:A:138:PHE:HA	2.17	0.43
1:E:177:PHE:CD2	2:E:404:C8E:H162	2.54	0.42
1:B:95:TYR:CE1	1:B:125:ARG:HG3	2.54	0.42
1:B:2:GLU:OE1	1:B:10:LYS:HD2	2.20	0.41
1:B:41:LYS:HE2	1:B:55:GLN:NE2	2.35	0.41
1:E:218:THR:HG22	1:E:239:THR:HG22	2.02	0.41
1:B:96:GLY:HA2	1:B:149:GLN:OE1	2.20	0.41
1:D:336:VAL:HG21	2:D:404:C8E:H71	2.01	0.41
1:E:295:TYR:CD2	1:E:315:LYS:HG3	2.56	0.41
1:E:338:LEU:HD23	1:E:338:LEU:HA	1.94	0.41
1:A:114:ASP:N	1:A:114:ASP:OD1	2.54	0.41
1:B:148:LEU:HD23	1:B:179:THR:HG22	2.03	0.41
1:F:246:GLY:HA3	1:F:328:ALA:HB1	2.03	0.41
1:B:295:TYR:CD2	1:B:315:LYS:HG3	2.56	0.41
1:E:114:ASP:N	1:E:114:ASP:OD1	2.53	0.41
1:E:296:VAL:HG23	1:E:318:LEU:HD11	2.01	0.41
1:B:48:ASP:HB3	1:B:49:GLN:NE2	2.26	0.40
1:D:283:LEU:HG	1:D:288:GLY:O	2.21	0.40
1:F:98:VAL:HB	1:F:123:GLN:HA	2.04	0.40
1:A:199:LYS:HD2	1:A:199:LYS:HA	1.79	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	338/345 (98%)	321 (95%)	17 (5%)	0	100	100
1	B	343/345 (99%)	323 (94%)	20 (6%)	0	100	100
1	C	338/345 (98%)	324 (96%)	13 (4%)	1 (0%)	43	37
1	D	343/345 (99%)	323 (94%)	20 (6%)	0	100	100
1	E	343/345 (99%)	323 (94%)	20 (6%)	0	100	100
1	F	343/345 (99%)	325 (95%)	17 (5%)	1 (0%)	43	37
All	All	2048/2070 (99%)	1939 (95%)	107 (5%)	2 (0%)	53	49

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	F	137	PHE
1	C	137	PHE

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	274/276 (99%)	270 (98%)	4 (2%)	67	70
1	B	276/276 (100%)	273 (99%)	3 (1%)	76	78
1	C	273/276 (99%)	270 (99%)	3 (1%)	76	78
1	D	276/276 (100%)	269 (98%)	7 (2%)	50	49
1	E	276/276 (100%)	271 (98%)	5 (2%)	62	63
1	F	276/276 (100%)	272 (99%)	4 (1%)	69	72
All	All	1651/1656 (100%)	1625 (98%)	26 (2%)	65	67

All (26) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	90	ASP
1	A	167	ARG
1	A	183	TYR

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Mol	Chain	Res	Type
1	A	235	GLN
1	B	83	PHE
1	B	90	ASP
1	B	167	ARG
1	C	90	ASP
1	C	167	ARG
1	C	235	GLN
1	D	10	LYS
1	D	82	LYS
1	D	90	ASP
1	D	167	ARG
1	D	183	TYR
1	D	235	GLN
1	D	326	ARG
1	E	90	ASP
1	E	167	ARG
1	E	187	ASP
1	E	224	LYS
1	E	266	ASP
1	F	64	ASN
1	F	90	ASP
1	F	167	ARG
1	F	321	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	49	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry

Of 35 ligands modelled in this entry, 6 are monoatomic - leaving 29 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	C8E	A	501	-	8,8,20	0.26	0	7,7,19	0.51	0
2	C8E	A	502	-	8,8,20	0.26	0	7,7,19	0.52	0
2	C8E	A	503	-	13,13,20	0.42	0	12,12,19	0.33	0
2	C8E	A	504	-	10,10,20	0.41	0	9,9,19	0.39	0
2	C8E	A	505	-	9,9,20	0.41	0	8,8,19	0.25	0
2	C8E	A	506	-	10,10,20	0.35	0	9,9,19	0.58	0
2	C8E	A	507	-	11,11,20	0.48	0	10,10,19	0.20	0
2	C8E	B	801	-	7,7,20	0.34	0	6,6,19	0.33	0
2	C8E	B	802	-	6,6,20	0.32	0	5,5,19	0.33	0
2	C8E	B	803	-	8,8,20	0.26	0	7,7,19	0.53	0
2	C8E	B	804	-	8,8,20	0.28	0	7,7,19	0.46	0
2	C8E	B	805	-	7,7,20	0.26	0	6,6,19	0.49	0
2	C8E	B	806	-	9,9,20	0.30	0	8,8,19	0.60	0
2	C8E	B	807	-	11,11,20	0.43	0	10,10,19	0.46	0
2	C8E	B	808	-	9,9,20	0.41	0	8,8,19	0.28	0
2	C8E	C	401	-	8,8,20	0.48	0	7,7,19	0.30	0
2	C8E	C	402	-	6,6,20	0.39	0	5,5,19	0.39	0
2	C8E	D	402	-	6,6,20	0.36	0	5,5,19	0.20	0
2	C8E	D	403	-	11,11,20	0.32	0	10,10,19	0.39	0
2	C8E	D	404	-	8,8,20	0.27	0	7,7,19	0.54	0
2	C8E	D	405	-	11,11,20	0.55	0	10,10,19	0.33	0
2	C8E	E	401	-	8,8,20	0.25	0	7,7,19	0.59	0
2	C8E	E	402	-	6,6,20	0.28	0	5,5,19	0.46	0
2	C8E	E	403	-	11,11,20	0.32	0	10,10,19	0.57	0
2	C8E	E	404	-	9,9,20	0.43	0	8,8,19	0.54	0
2	C8E	E	405	-	5,5,20	0.29	0	4,4,19	0.40	0
2	C8E	F	401	-	7,7,20	0.28	0	6,6,19	0.46	0
2	C8E	F	402	-	7,7,20	0.40	0	6,6,19	0.16	0
2	C8E	F	403	-	15,15,20	0.49	0	14,14,19	0.30	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the

Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns.
'-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	C8E	A	501	-	-	5/6/6/18	-
2	C8E	A	502	-	-	2/6/6/18	-
2	C8E	A	503	-	-	9/11/11/18	-
2	C8E	A	504	-	-	5/8/8/18	-
2	C8E	A	505	-	-	7/7/7/18	-
2	C8E	A	506	-	-	3/8/8/18	-
2	C8E	A	507	-	-	7/9/9/18	-
2	C8E	B	801	-	-	3/5/5/18	-
2	C8E	B	802	-	-	0/4/4/18	-
2	C8E	B	803	-	-	2/6/6/18	-
2	C8E	B	804	-	-	3/6/6/18	-
2	C8E	B	805	-	-	3/5/5/18	-
2	C8E	B	806	-	-	6/7/7/18	-
2	C8E	B	807	-	-	5/9/9/18	-
2	C8E	B	808	-	-	5/7/7/18	-
2	C8E	C	401	-	-	5/6/6/18	-
2	C8E	C	402	-	-	2/4/4/18	-
2	C8E	D	402	-	-	2/4/4/18	-
2	C8E	D	403	-	-	4/9/9/18	-
2	C8E	D	404	-	-	4/6/6/18	-
2	C8E	D	405	-	-	6/9/9/18	-
2	C8E	E	401	-	-	1/6/6/18	-
2	C8E	E	402	-	-	3/4/4/18	-
2	C8E	E	403	-	-	7/9/9/18	-
2	C8E	E	404	-	-	5/7/7/18	-
2	C8E	E	405	-	-	1/3/3/18	-
2	C8E	F	401	-	-	3/5/5/18	-
2	C8E	F	402	-	-	2/5/5/18	-
2	C8E	F	403	-	-	10/13/13/18	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (120) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	503	C8E	C16-C17-O18-C19
2	A	503	C8E	O12-C13-C14-O15
2	A	504	C8E	O12-C13-C14-O15
2	A	504	C8E	O15-C16-C17-O18
2	F	403	C8E	C6-C7-C8-O9
2	B	801	C8E	C7-C8-O9-C10
2	D	405	C8E	O15-C16-C17-O18
2	F	403	C8E	C17-C16-O15-C14
2	B	807	C8E	O15-C16-C17-O18
2	A	507	C8E	O12-C13-C14-O15
2	B	807	C8E	O12-C13-C14-O15
2	A	503	C8E	O15-C16-C17-O18
2	C	401	C8E	O18-C19-C20-O21
2	A	505	C8E	O12-C13-C14-O15
2	F	403	C8E	O12-C13-C14-O15
2	B	807	C8E	O18-C19-C20-O21
2	C	402	C8E	O15-C16-C17-O18
2	C	402	C8E	O18-C19-C20-O21
2	E	404	C8E	O12-C13-C14-O15
2	E	404	C8E	O18-C19-C20-O21
2	B	808	C8E	C7-C8-O9-C10
2	E	402	C8E	C3-C4-C5-C6
2	E	403	C8E	C2-C3-C4-C5
2	A	501	C8E	C2-C3-C4-C5
2	B	808	C8E	C4-C5-C6-C7
2	B	803	C8E	C2-C3-C4-C5
2	E	403	C8E	C3-C4-C5-C6
2	B	804	C8E	C3-C4-C5-C6
2	A	502	C8E	C2-C3-C4-C5
2	B	808	C8E	C3-C4-C5-C6
2	D	405	C8E	O12-C13-C14-O15
2	B	806	C8E	C5-C6-C7-C8
2	E	405	C8E	C3-C4-C5-C6
2	A	507	C8E	O18-C19-C20-O21
2	D	403	C8E	C3-C4-C5-C6
2	A	507	C8E	O15-C16-C17-O18
2	E	403	C8E	C4-C5-C6-C7
2	E	404	C8E	C16-C17-O18-C19
2	B	806	C8E	C2-C3-C4-C5
2	A	506	C8E	C1-C2-C3-C4
2	A	501	C8E	C6-C7-C8-O9
2	A	504	C8E	O18-C19-C20-O21
2	D	405	C8E	O18-C19-C20-O21

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Mol	Chain	Res	Type	Atoms
2	F	403	C8E	O9-C10-C11-O12
2	D	404	C8E	C3-C4-C5-C6
2	E	403	C8E	C1-C2-C3-C4
2	B	803	C8E	C6-C7-C8-O9
2	B	808	C8E	C6-C7-C8-O9
2	B	801	C8E	C4-C5-C6-C7
2	E	402	C8E	C4-C5-C6-C7
2	D	404	C8E	C5-C6-C7-C8
2	A	501	C8E	C3-C4-C5-C6
2	B	807	C8E	C10-C11-O12-C13
2	A	505	C8E	C17-C16-O15-C14
2	A	502	C8E	C1-C2-C3-C4
2	B	806	C8E	C7-C8-O9-C10
2	B	806	C8E	C3-C4-C5-C6
2	B	804	C8E	C1-C2-C3-C4
2	B	801	C8E	C6-C7-C8-O9
2	F	401	C8E	C2-C3-C4-C5
2	B	808	C8E	C5-C6-C7-C8
2	B	805	C8E	C2-C3-C4-C5
2	A	503	C8E	C10-C11-O12-C13
2	C	401	C8E	C13-C14-O15-C16
2	B	807	C8E	C14-C13-O12-C11
2	A	505	C8E	C16-C17-O18-C19
2	D	405	C8E	C20-C19-O18-C17
2	A	503	C8E	C13-C14-O15-C16
2	F	403	C8E	C14-C13-O12-C11
2	D	405	C8E	C13-C14-O15-C16
2	D	405	C8E	C16-C17-O18-C19
2	A	507	C8E	C16-C17-O18-C19
2	C	401	C8E	C17-C16-O15-C14
2	F	403	C8E	C7-C8-O9-C10
2	D	403	C8E	C1-C2-C3-C4
2	F	403	C8E	C13-C14-O15-C16
2	F	402	C8E	C20-C19-O18-C17
2	E	403	C8E	C7-C8-O9-C10
2	A	506	C8E	C7-C8-O9-C10
2	F	403	C8E	O15-C16-C17-O18
2	A	507	C8E	C20-C19-O18-C17
2	A	507	C8E	C17-C16-O15-C14
2	F	401	C8E	C1-C2-C3-C4
2	E	402	C8E	C2-C3-C4-C5
2	F	403	C8E	C20-C19-O18-C17

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Mol	Chain	Res	Type	Atoms
2	A	503	C8E	C14-C13-O12-C11
2	A	504	C8E	C14-C13-O12-C11
2	A	501	C8E	C1-C2-C3-C4
2	B	806	C8E	C1-C2-C3-C4
2	D	404	C8E	C6-C7-C8-O9
2	A	504	C8E	C17-C16-O15-C14
2	A	503	C8E	O18-C19-C20-O21
2	A	503	C8E	C17-C16-O15-C14
2	A	505	C8E	C20-C19-O18-C17
2	A	505	C8E	O18-C19-C20-O21
2	B	806	C8E	C4-C5-C6-C7
2	B	804	C8E	C2-C3-C4-C5
2	A	503	C8E	C20-C19-O18-C17
2	D	402	C8E	C7-C8-O9-C10
2	D	404	C8E	C4-C5-C6-C7
2	D	402	C8E	C6-C7-C8-O9
2	B	805	C8E	C3-C4-C5-C6
2	C	401	C8E	C20-C19-O18-C17
2	E	403	C8E	O9-C10-C11-O12
2	E	403	C8E	C6-C7-C8-O9
2	E	401	C8E	C3-C4-C5-C6
2	F	403	C8E	C11-C10-O9-C8
2	D	403	C8E	O9-C10-C11-O12
2	F	401	C8E	C4-C5-C6-C7
2	A	507	C8E	C13-C14-O15-C16
2	F	402	C8E	O15-C16-C17-O18
2	A	506	C8E	C3-C4-C5-C6
2	B	805	C8E	C4-C5-C6-C7
2	A	505	C8E	O15-C16-C17-O18
2	A	501	C8E	C4-C5-C6-C7
2	C	401	C8E	O15-C16-C17-O18
2	E	404	C8E	O15-C16-C17-O18
2	A	505	C8E	C13-C14-O15-C16
2	D	403	C8E	C2-C3-C4-C5
2	E	404	C8E	C17-C16-O15-C14

There are no ring outliers.

7 monomers are involved in 9 short contacts:

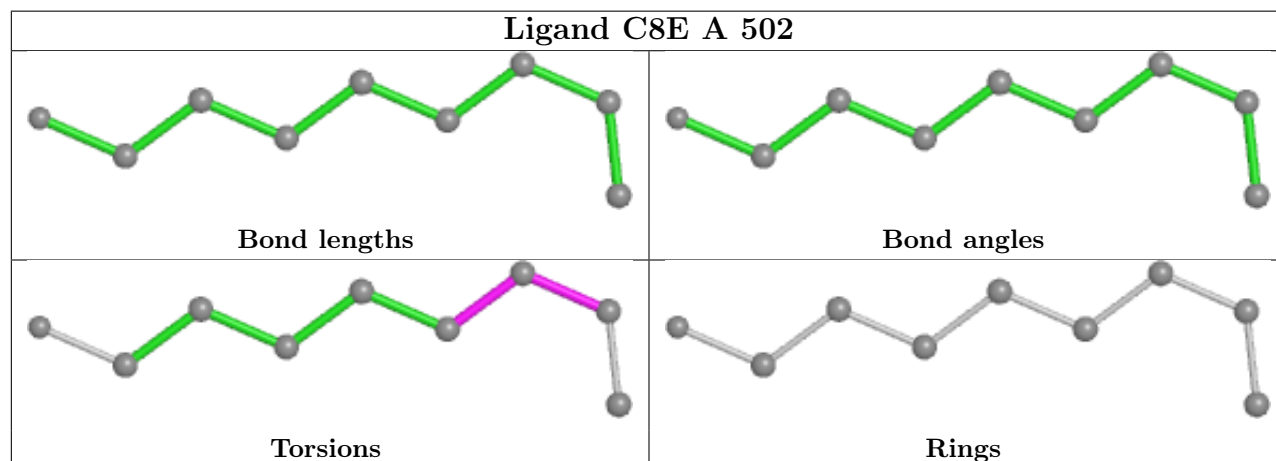
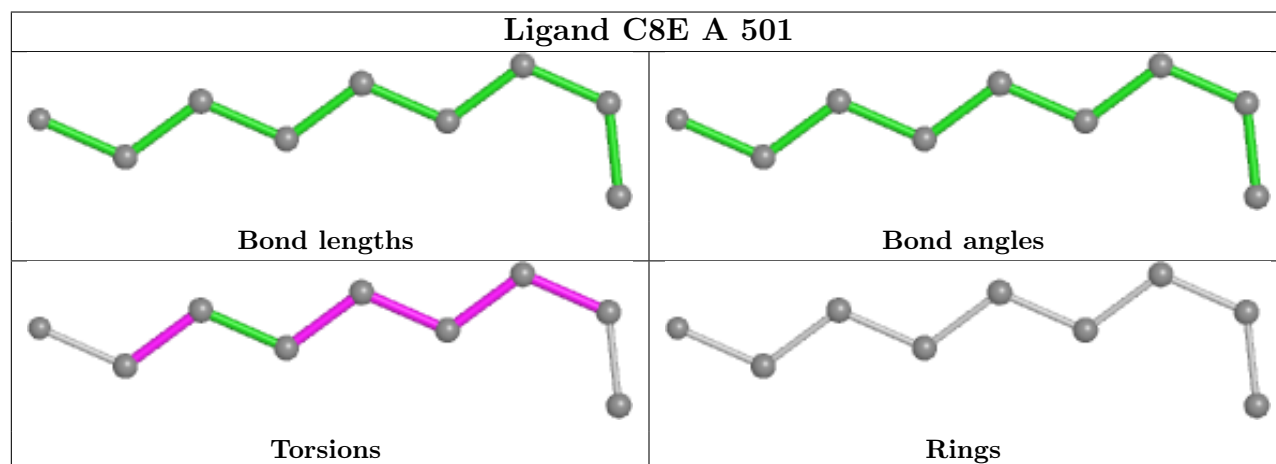
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	503	C8E	1	0
2	A	505	C8E	1	0

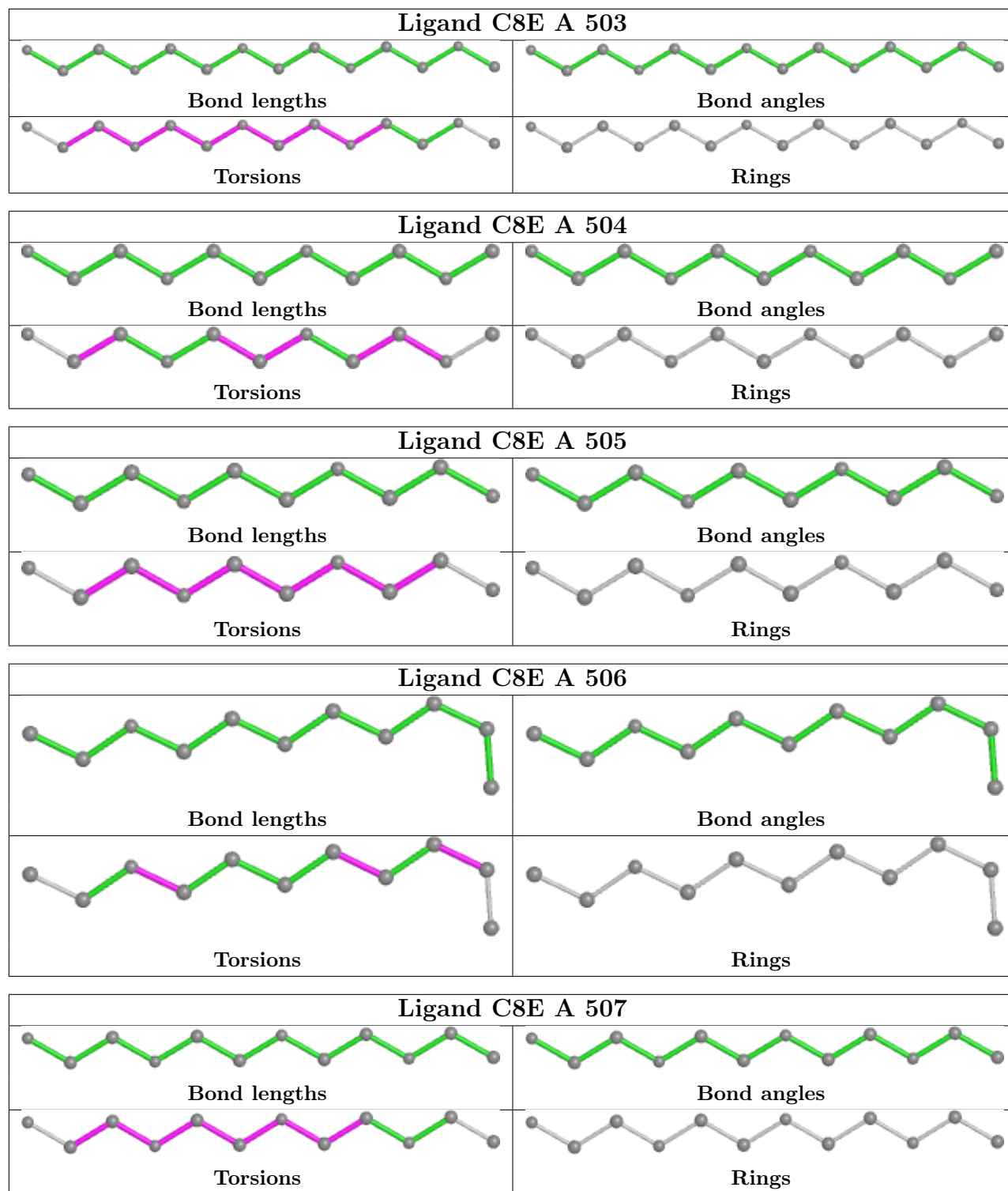
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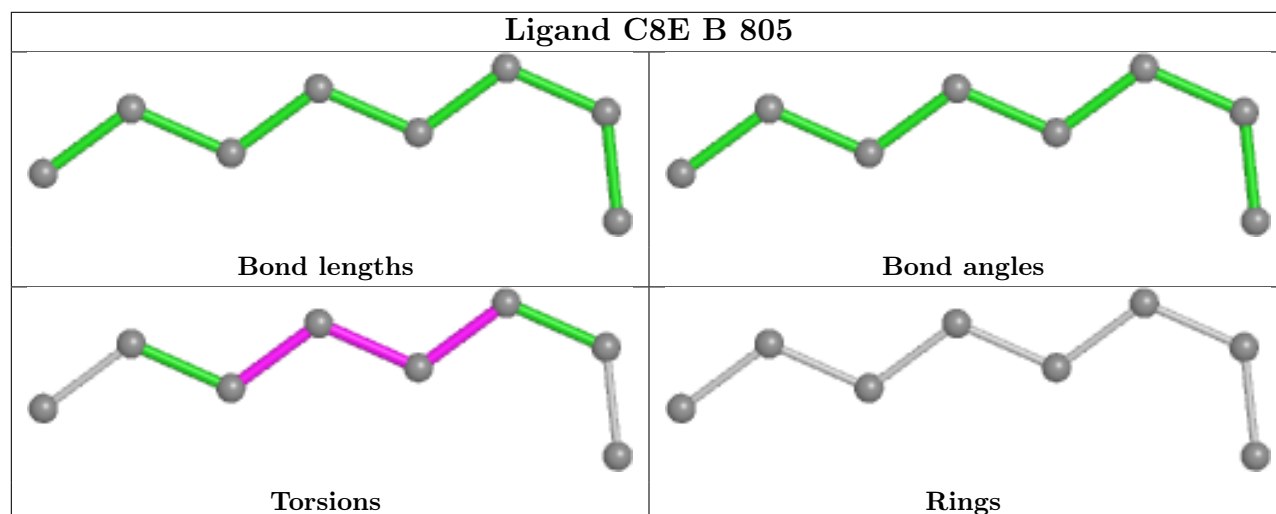
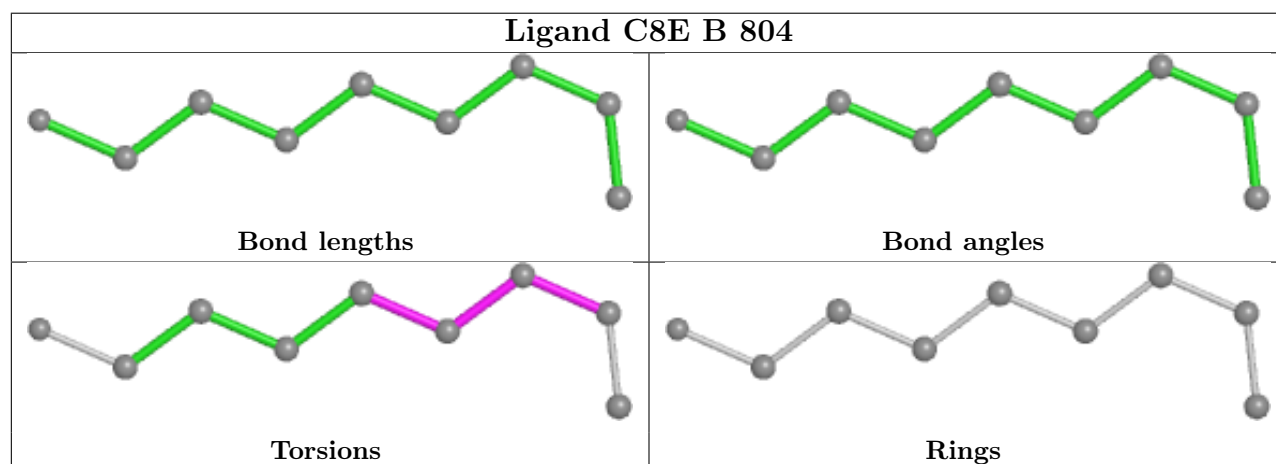
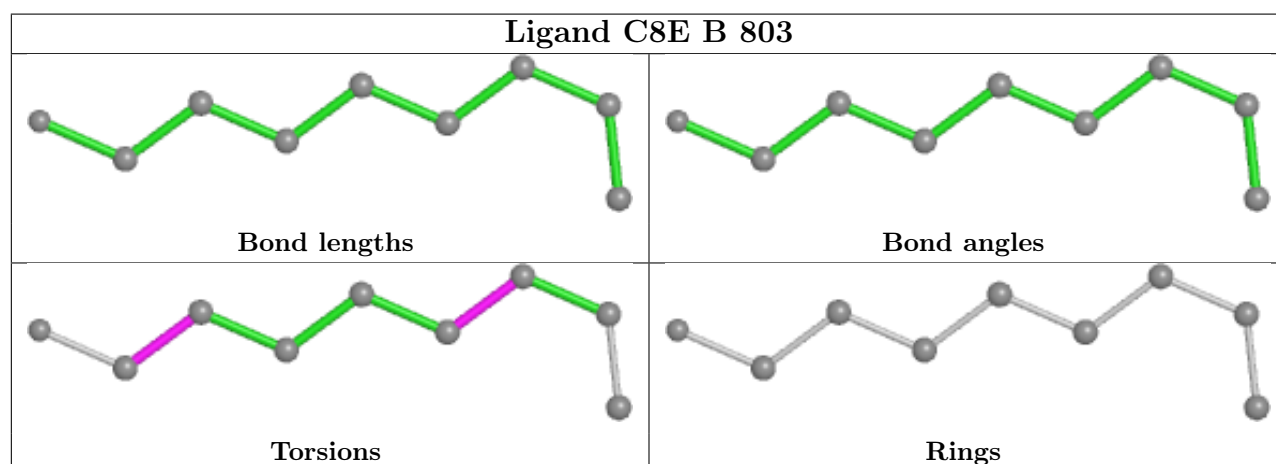
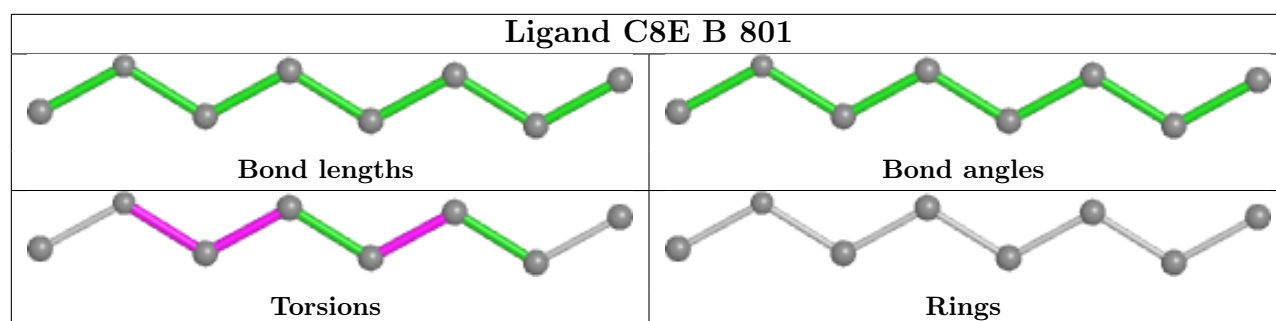
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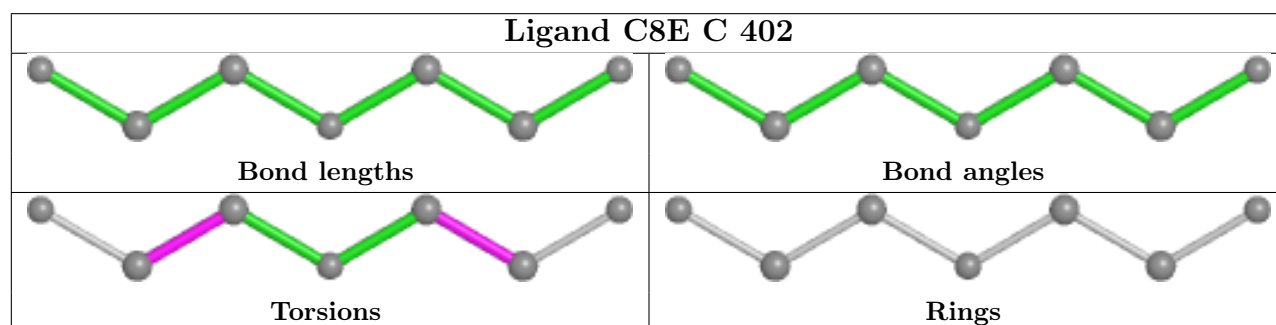
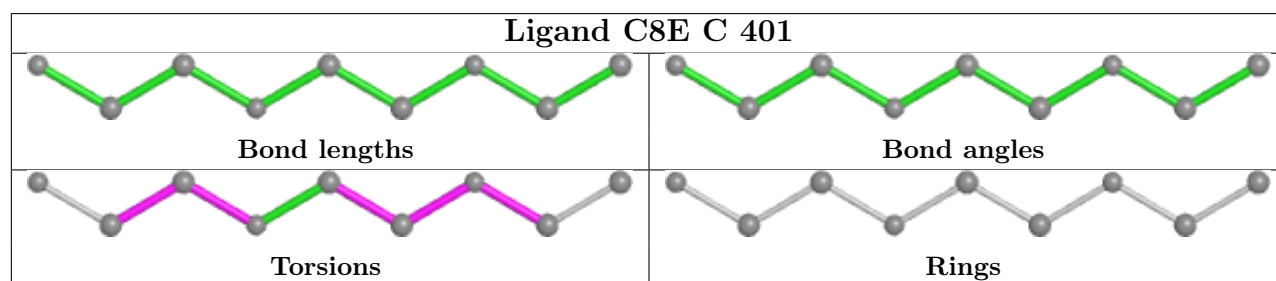
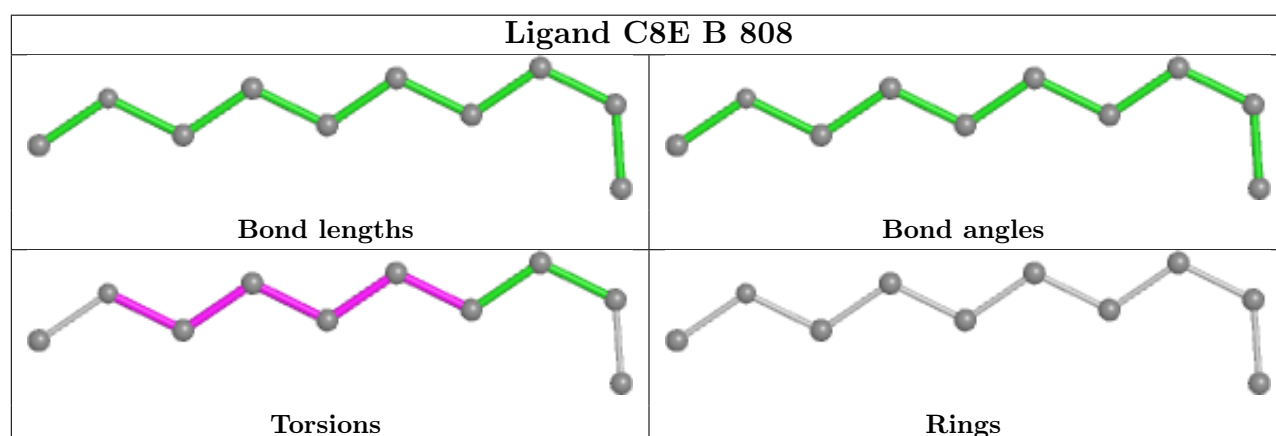
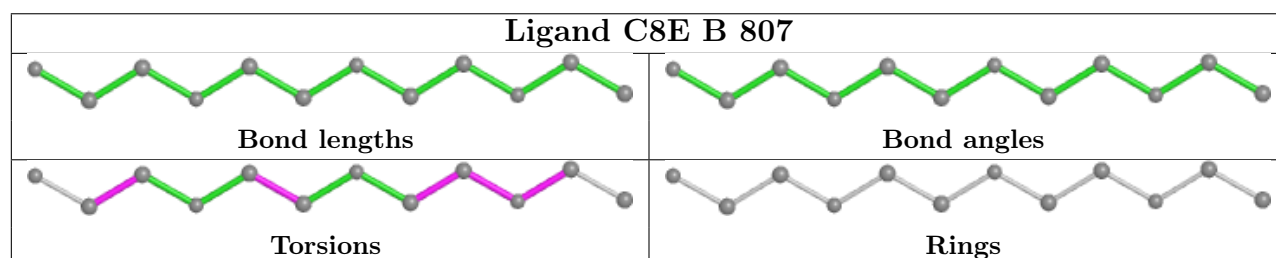
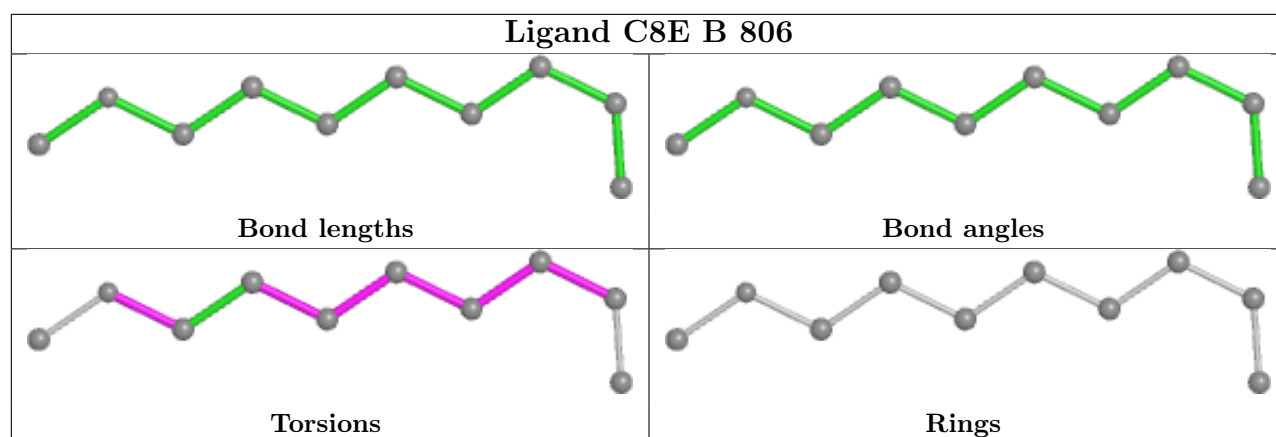
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	506	C8E	1	0
2	B	801	C8E	1	0
2	D	404	C8E	1	0
2	D	405	C8E	2	0
2	E	404	C8E	2	0

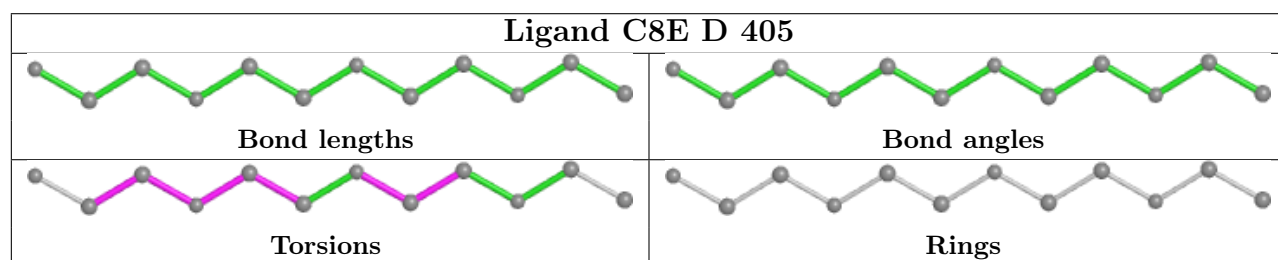
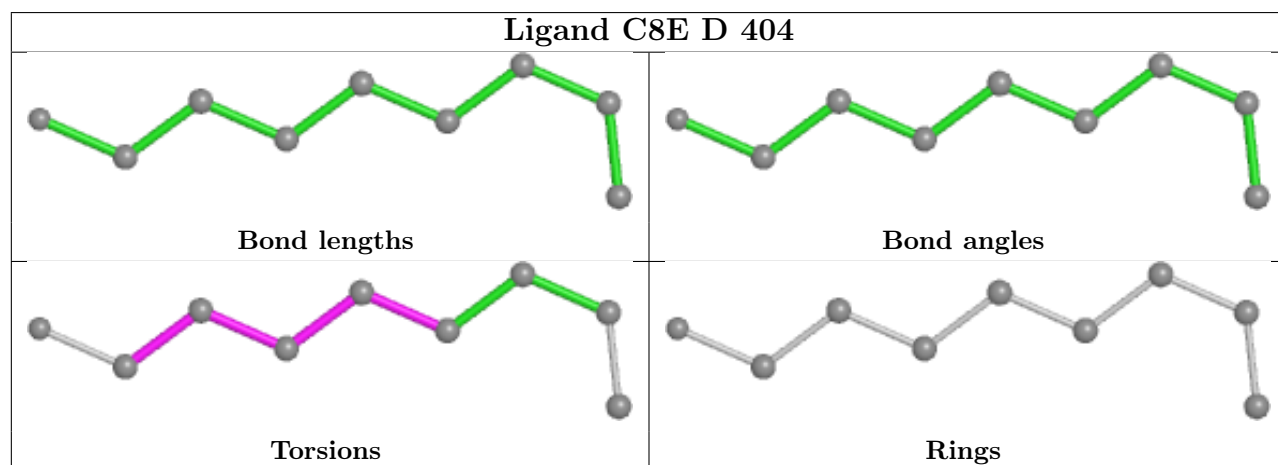
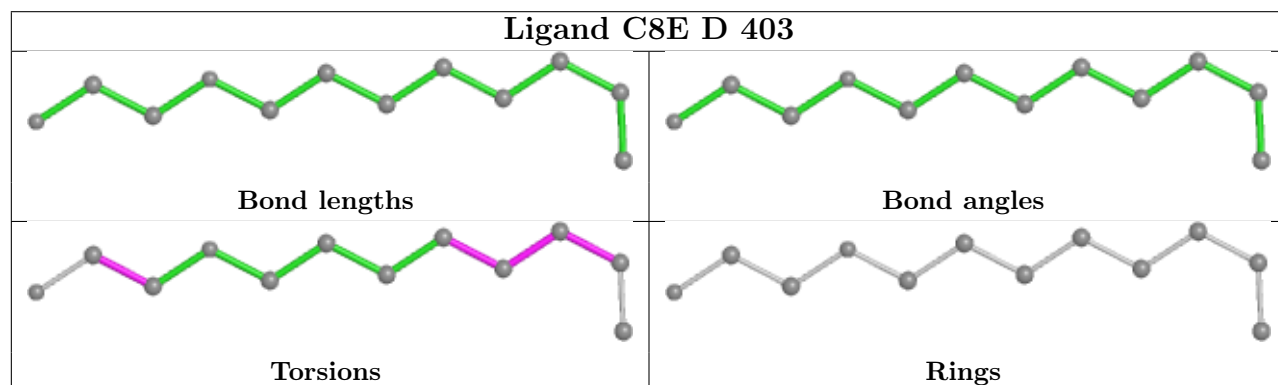
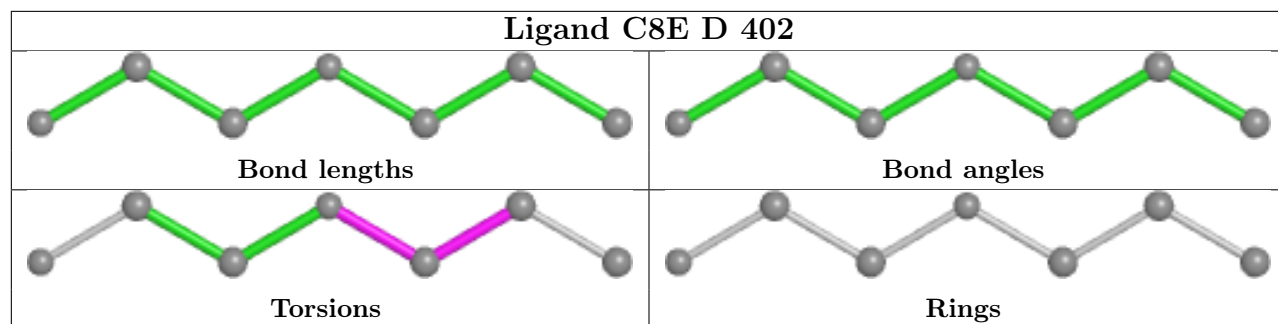
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

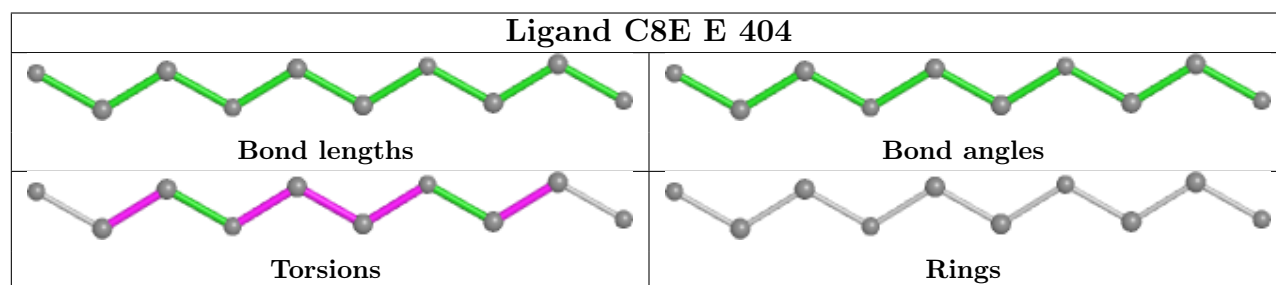
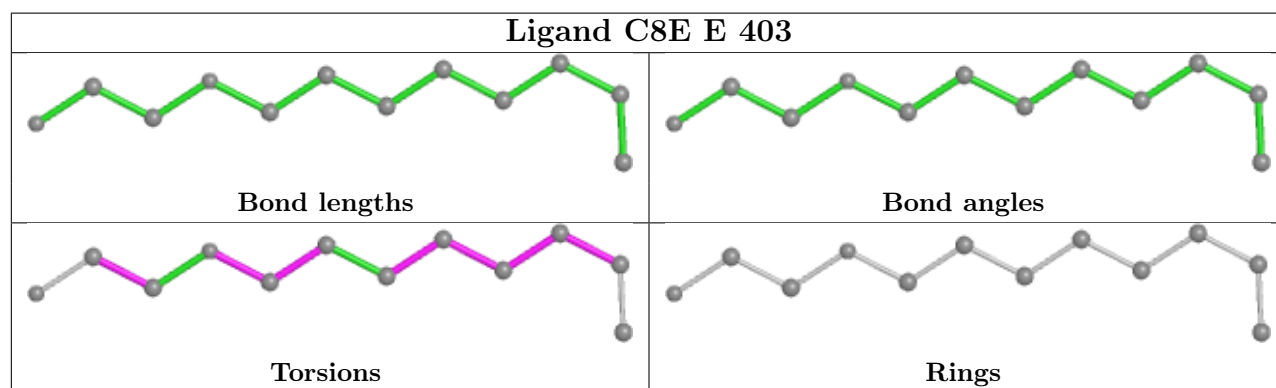
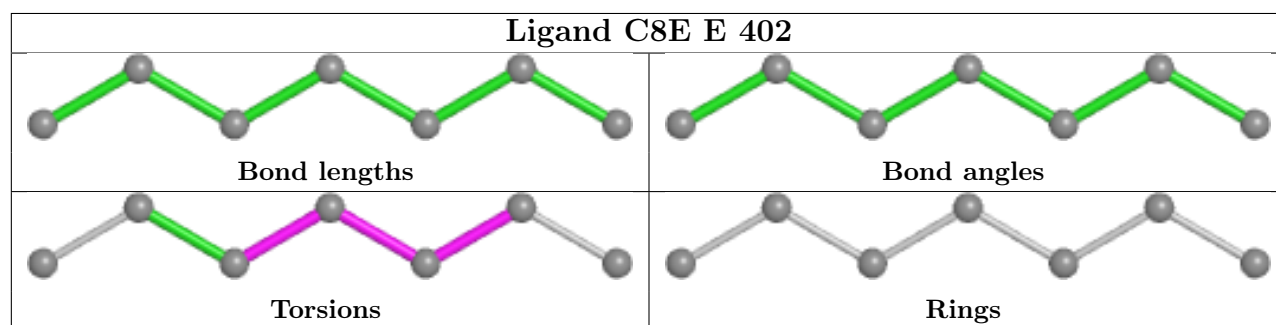
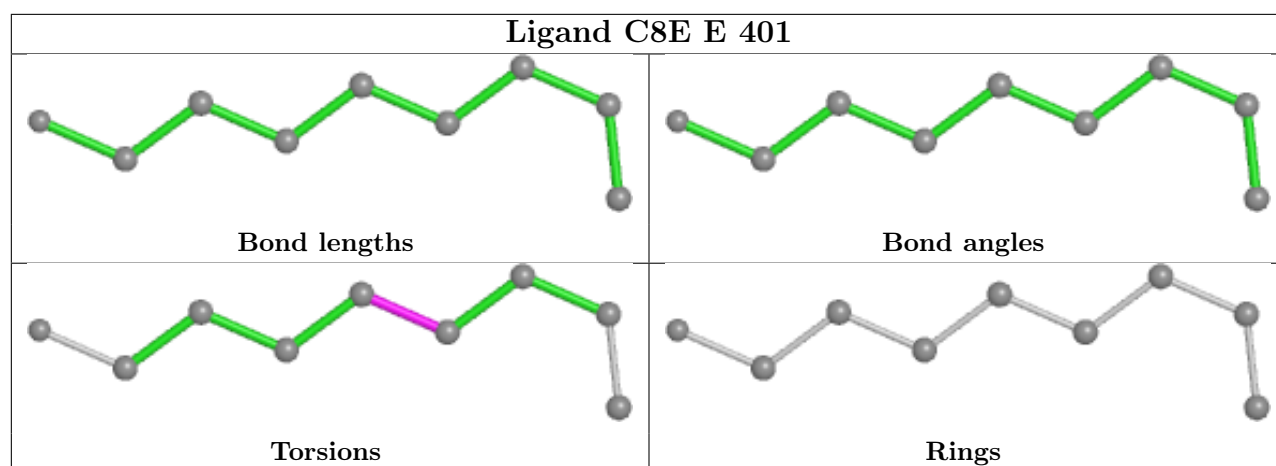


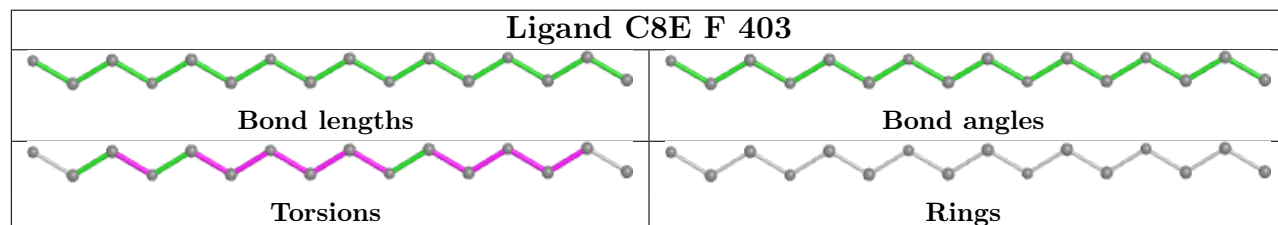
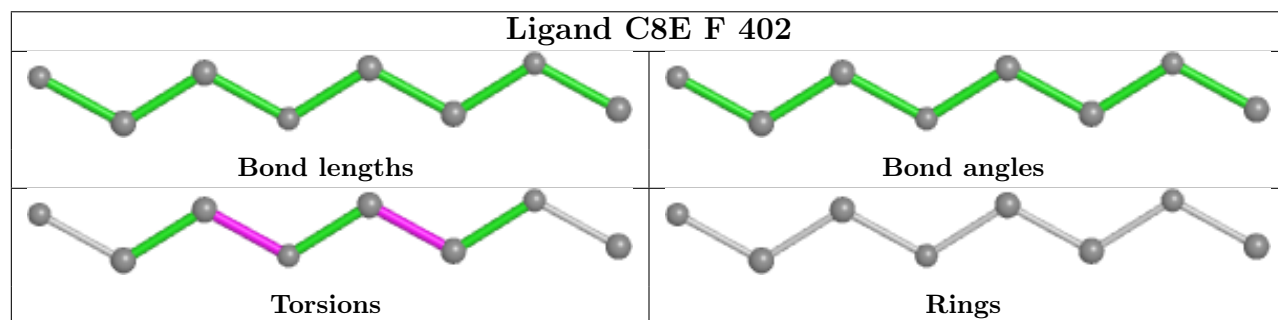
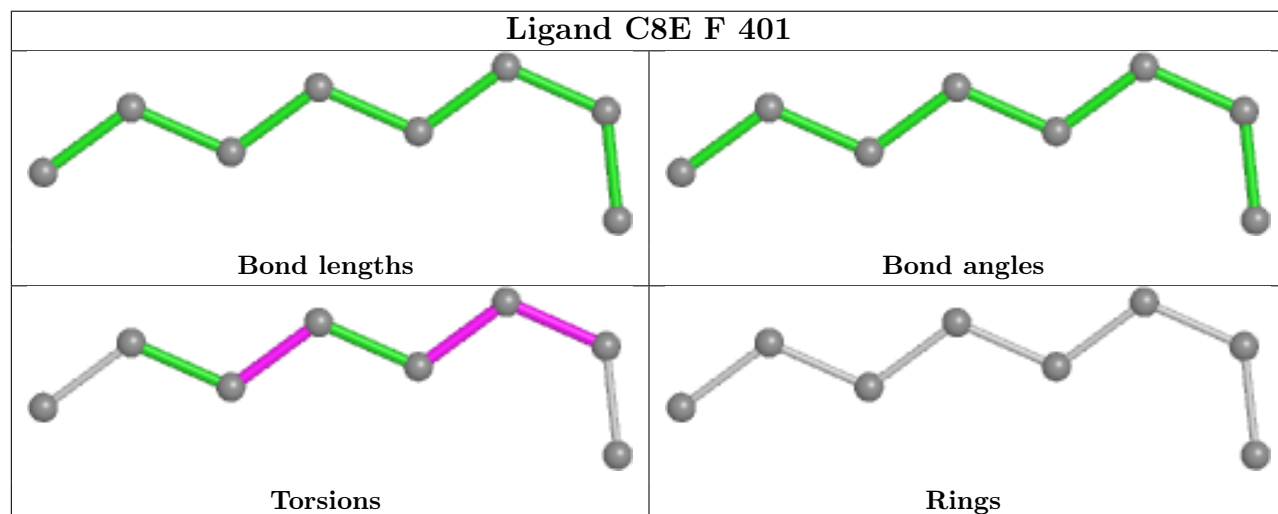
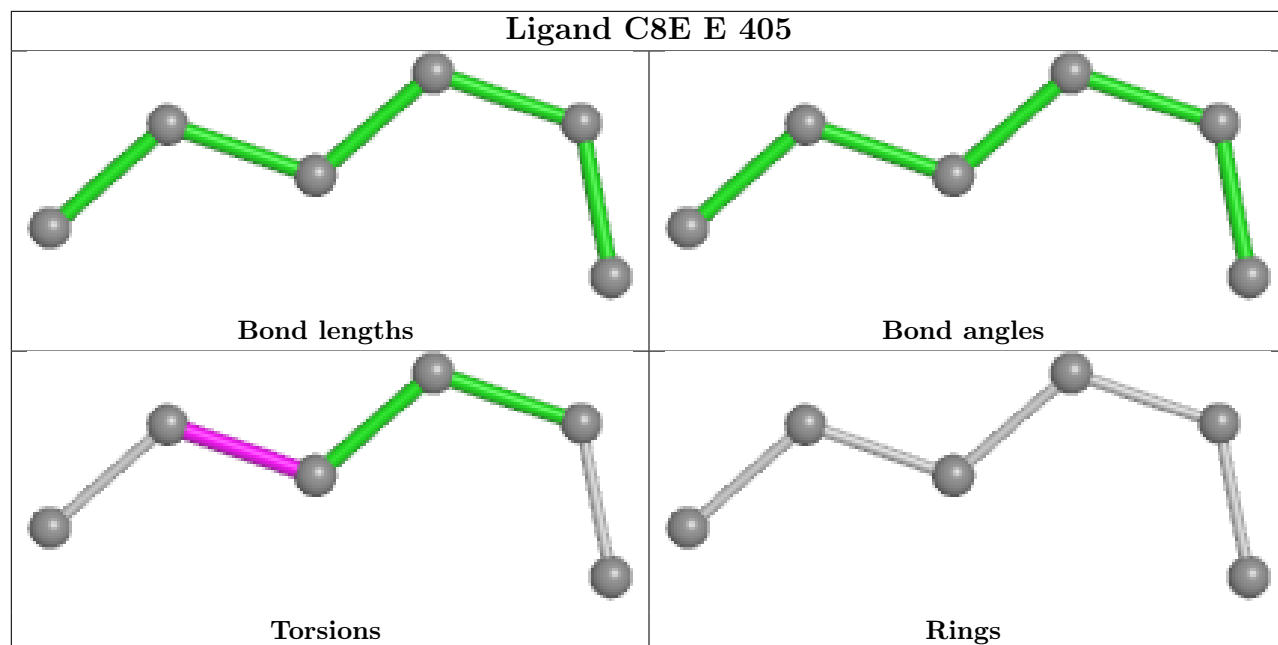












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	342/345 (99%)	-0.11	2 (0%) 89 90	16, 23, 32, 41	0
1	B	345/345 (100%)	-0.08	3 (0%) 84 85	17, 22, 35, 69	0
1	C	342/345 (99%)	-0.06	2 (0%) 89 90	17, 23, 34, 44	0
1	D	345/345 (100%)	-0.13	6 (1%) 70 71	17, 22, 32, 48	0
1	E	345/345 (100%)	-0.07	6 (1%) 70 71	17, 24, 34, 67	0
1	F	345/345 (100%)	-0.03	6 (1%) 70 71	16, 24, 34, 74	0
All	All	2064/2070 (99%)	-0.08	25 (1%) 79 80	16, 23, 34, 74	0

All (25) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	186	TRP	9.2
1	E	186	TRP	7.5
1	B	186	TRP	7.2
1	B	185	ILE	5.7
1	F	187	ASP	5.4
1	E	187	ASP	3.3
1	D	187	ASP	3.1
1	D	186	TRP	3.0
1	E	321	ASP	2.7
1	C	150	TYR	2.7
1	D	48	ASP	2.6
1	E	193	PHE	2.4
1	D	193	PHE	2.3
1	E	282	ASP	2.3
1	A	83	PHE	2.2
1	F	83	PHE	2.2
1	D	49	GLN	2.2
1	F	287	TYR	2.2
1	F	286	GLY	2.2

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Mol	Chain	Res	Type	RSRZ
1	E	185	ILE	2.2
1	C	227	ALA	2.2
1	F	185	ILE	2.1
1	D	6	LYS	2.1
1	B	48	ASP	2.0
1	A	160	GLU	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	C8E	C	401	9/21	0.72	0.18	35,37,43,43	0
2	C8E	A	506	11/21	0.73	0.23	25,30,42,45	0
2	C8E	E	403	12/21	0.77	0.17	31,34,45,51	0
2	C8E	B	808	10/21	0.79	0.15	24,34,38,46	0
2	C8E	B	803	9/21	0.79	0.15	30,37,43,49	0
2	C8E	F	403	16/21	0.81	0.14	25,36,42,43	0
2	C8E	B	801	8/21	0.81	0.17	31,37,45,51	0
2	C8E	A	505	10/21	0.81	0.17	37,43,52,53	0
2	C8E	B	806	10/21	0.81	0.15	25,33,41,41	0
2	C8E	F	402	8/21	0.82	0.23	40,41,46,48	0
2	C8E	D	405	12/21	0.82	0.18	27,37,42,43	0
2	C8E	E	405	6/21	0.83	0.16	31,31,35,38	0
2	C8E	D	404	9/21	0.84	0.20	35,38,43,48	0
2	C8E	A	507	12/21	0.84	0.25	37,43,48,50	0
2	C8E	C	402	7/21	0.85	0.15	27,33,36,38	0
2	C8E	D	402	7/21	0.85	0.14	26,31,37,41	0
2	C8E	A	504	11/21	0.86	0.13	28,36,41,44	0

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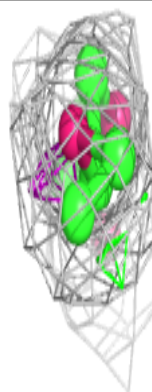
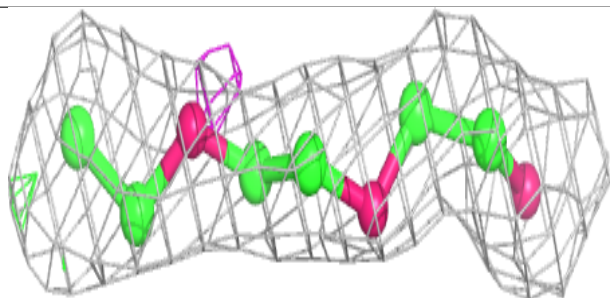
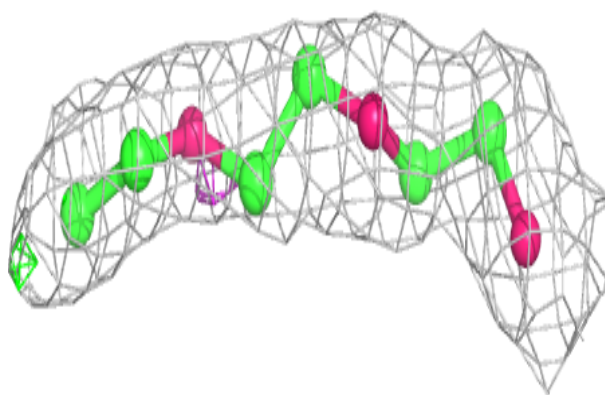
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	C8E	E	402	7/21	0.88	0.15	24,31,34,34	0
2	C8E	B	807	12/21	0.88	0.15	26,35,43,49	0
2	C8E	D	403	12/21	0.88	0.12	28,34,37,44	0
2	C8E	A	502	9/21	0.88	0.16	21,26,34,41	0
2	C8E	E	401	9/21	0.90	0.11	28,31,36,41	0
2	C8E	A	503	14/21	0.90	0.12	31,34,40,41	0
2	C8E	B	802	7/21	0.91	0.12	25,27,31,31	0
2	C8E	B	805	8/21	0.91	0.10	27,30,35,35	0
2	C8E	A	501	9/21	0.92	0.10	24,28,30,34	0
2	C8E	F	401	8/21	0.92	0.17	23,28,31,31	0
2	C8E	B	804	9/21	0.93	0.15	25,28,34,42	0
3	MG	B	809	1/1	0.94	0.21	33,33,33,33	0
3	MG	F	404	1/1	0.94	0.25	29,29,29,29	0
2	C8E	E	404	10/21	0.94	0.11	26,34,37,38	0
3	MG	C	403	1/1	0.97	0.17	24,24,24,24	0
3	MG	A	508	1/1	0.97	0.20	23,23,23,23	0
3	MG	E	406	1/1	0.97	0.24	36,36,36,36	0
3	MG	D	401	1/1	0.99	0.15	21,21,21,21	0

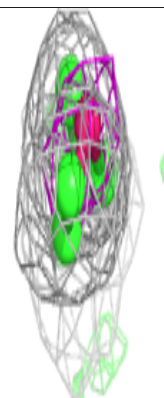
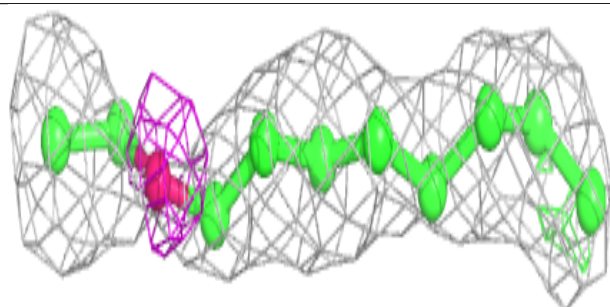
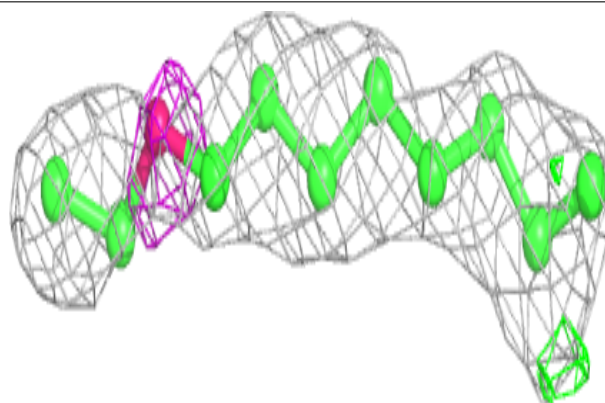
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around C8E C 401:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

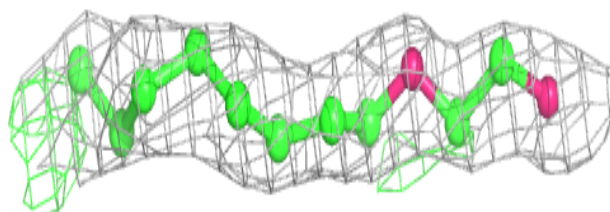
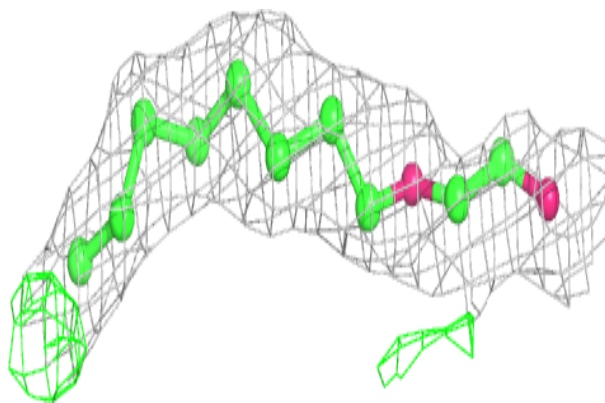
**Electron density around C8E A 506:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

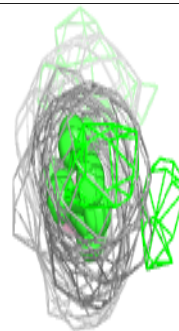
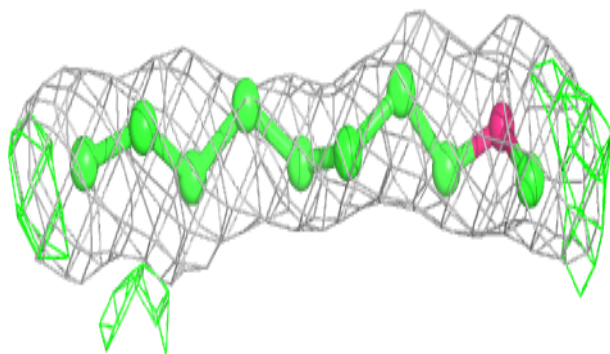
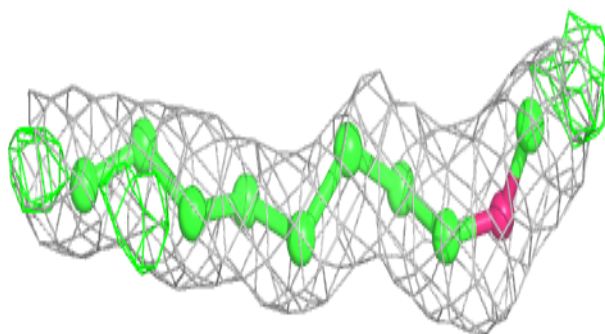


Electron density around C8E E 403:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

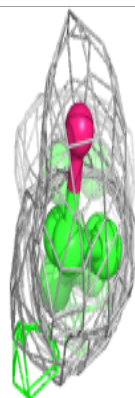
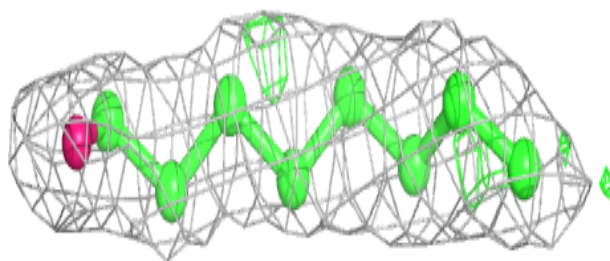
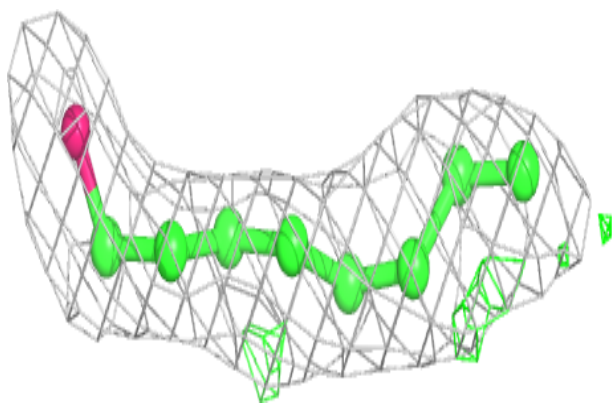
**Electron density around C8E B 808:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

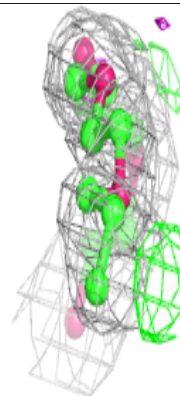
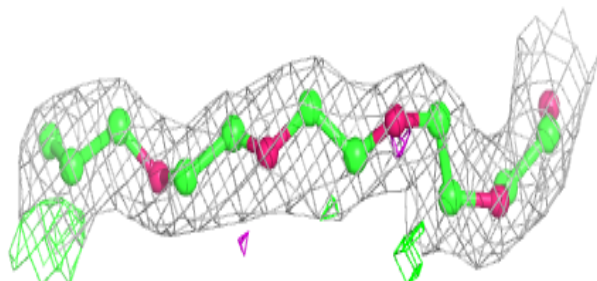
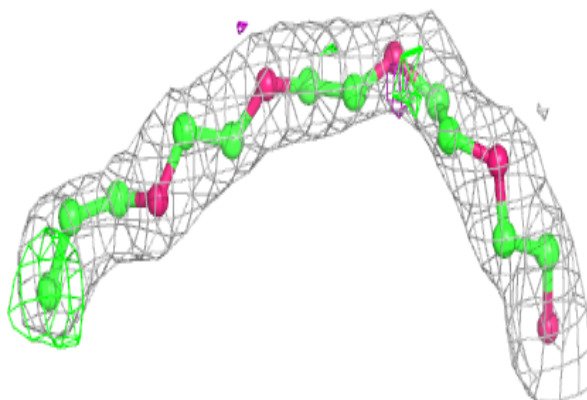


Electron density around C8E B 803:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

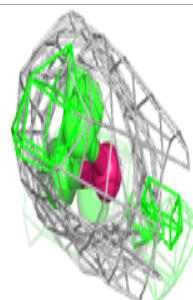
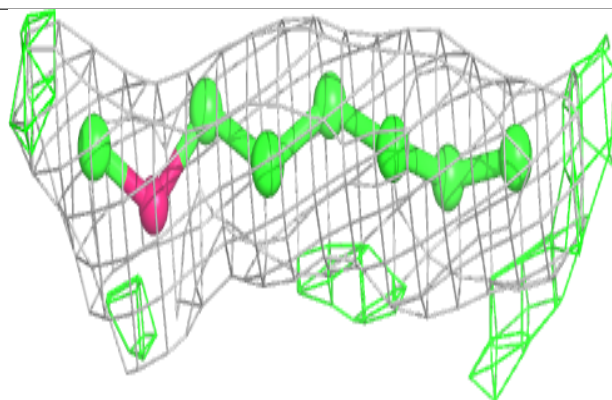
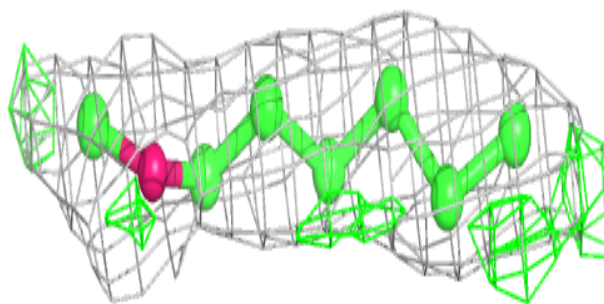
**Electron density around C8E F 403:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

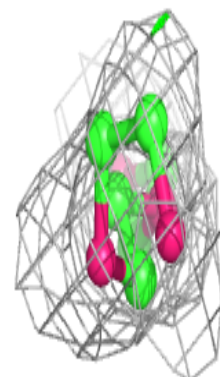
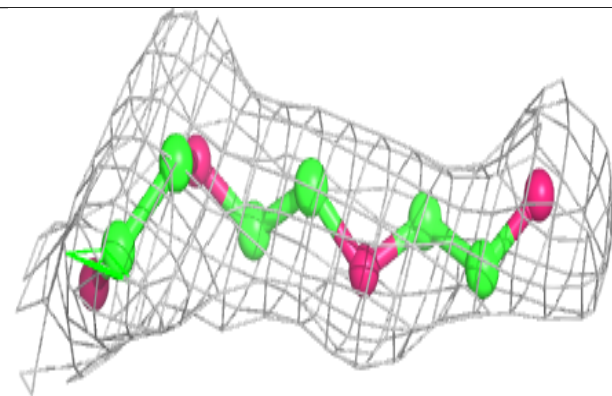
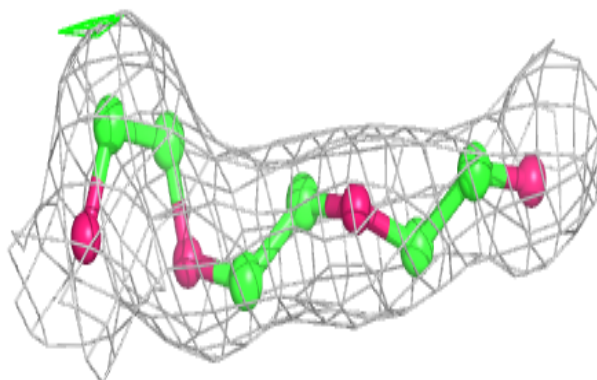


Electron density around C8E B 801:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

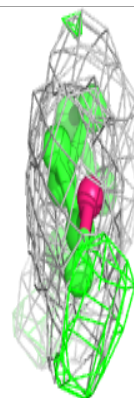
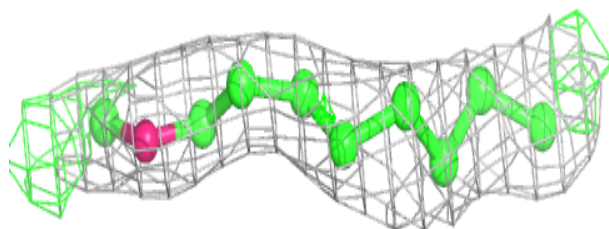
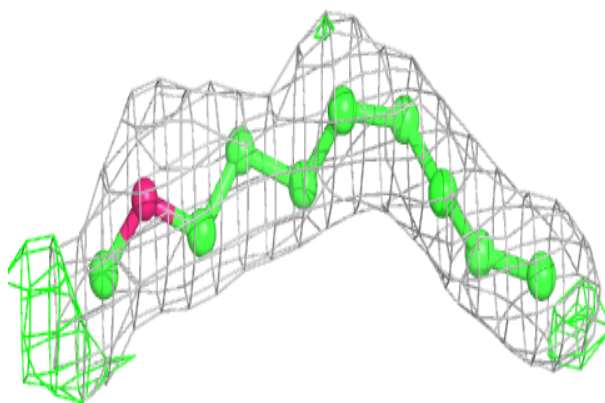
**Electron density around C8E A 505:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

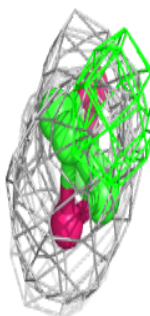
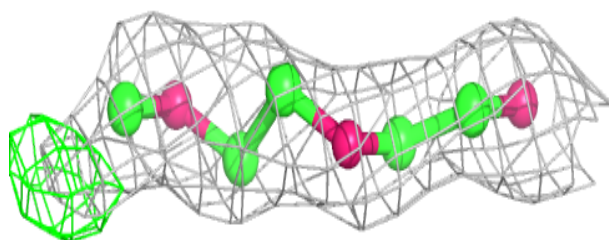
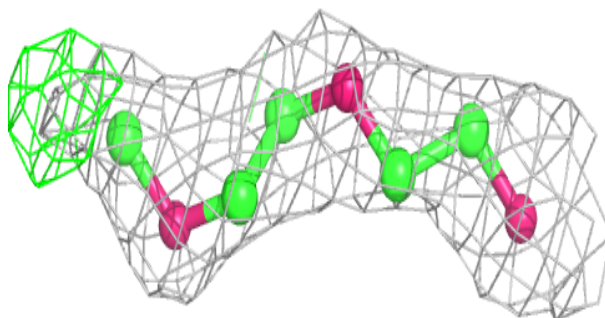


Electron density around C8E B 806:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

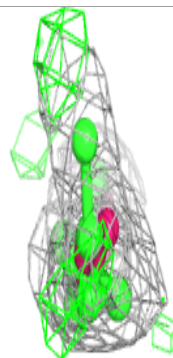
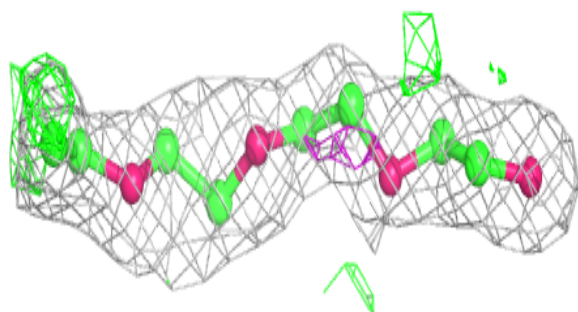
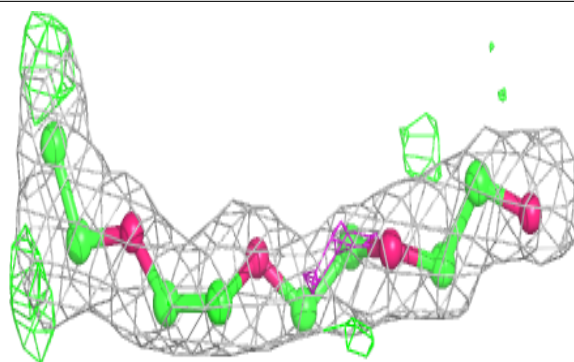
**Electron density around C8E F 402:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



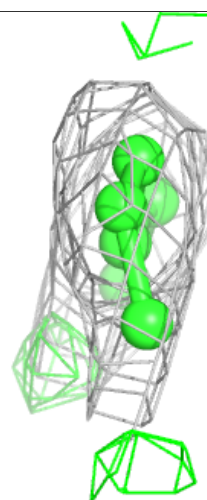
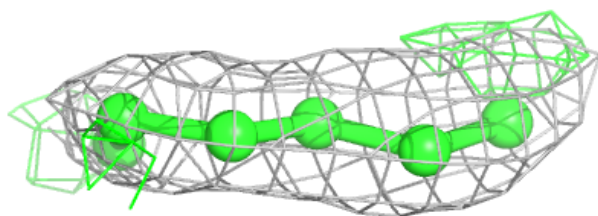
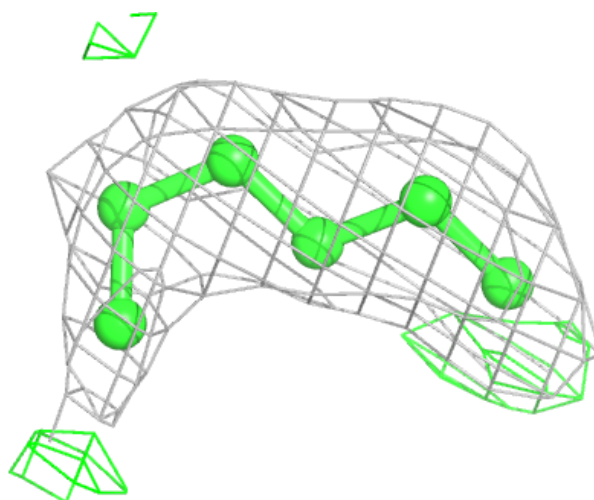
Electron density around C8E D 405:

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



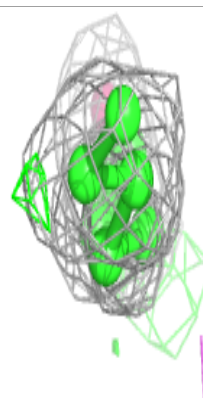
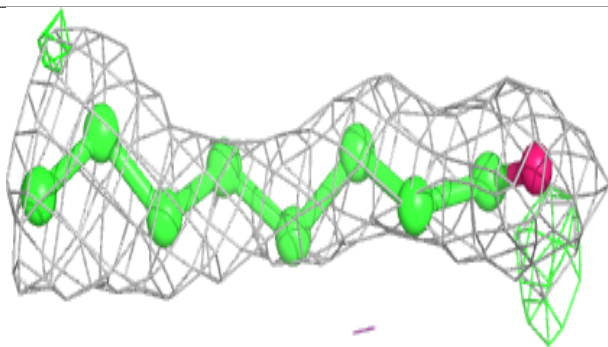
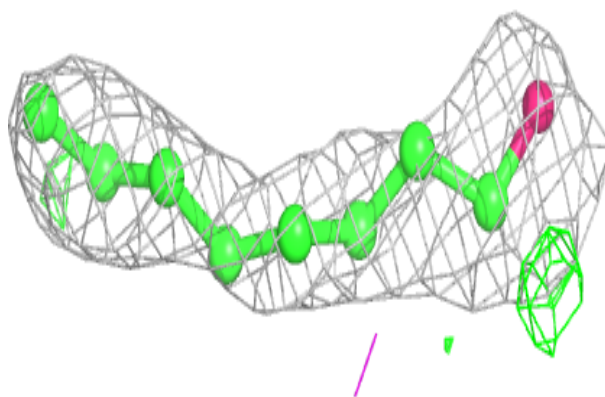
Electron density around C8E E 405:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

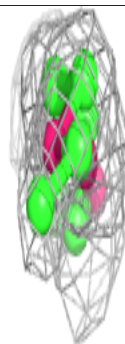
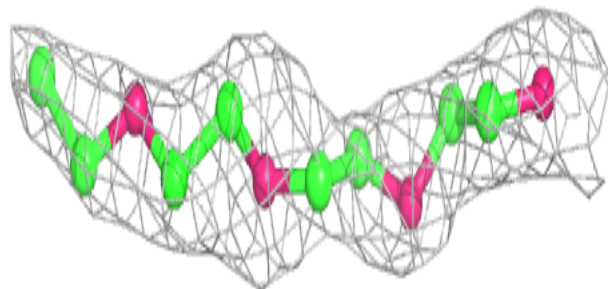
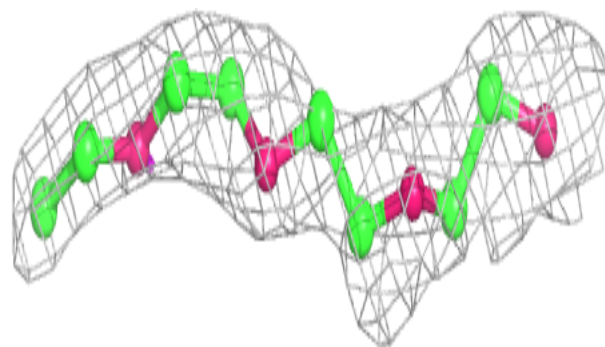


Electron density around C8E D 404:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

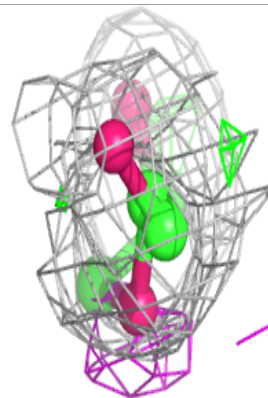
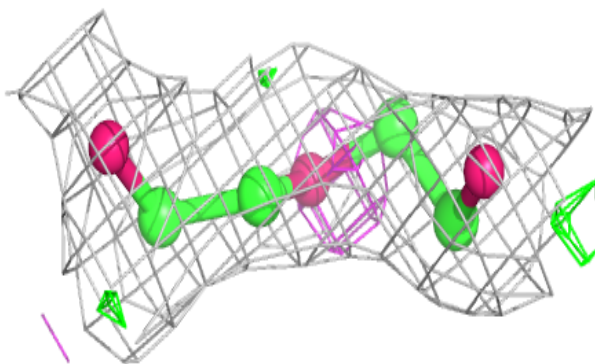
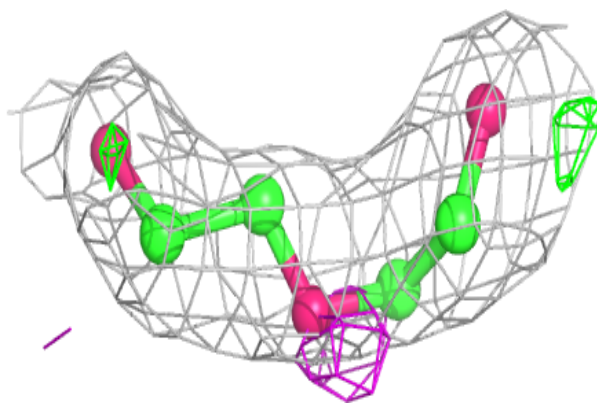
**Electron density around C8E A 507:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

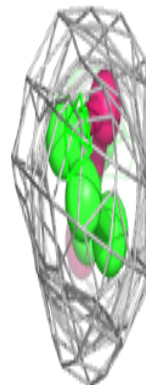
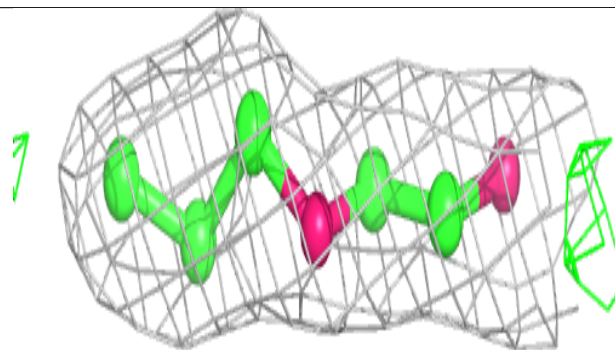
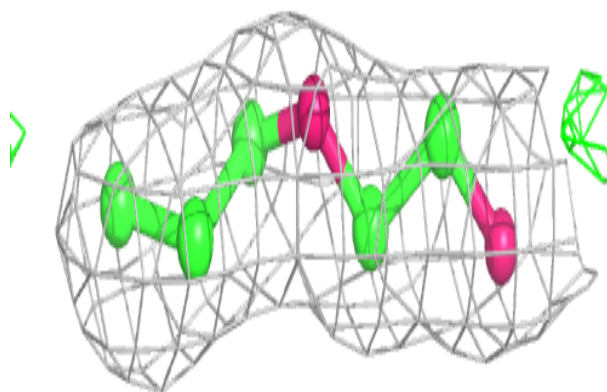


Electron density around C8E C 402:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

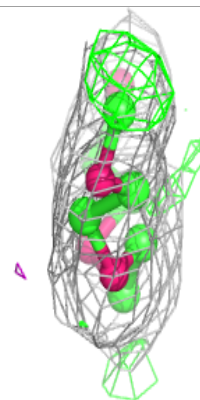
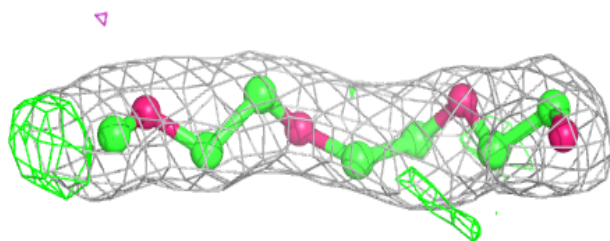
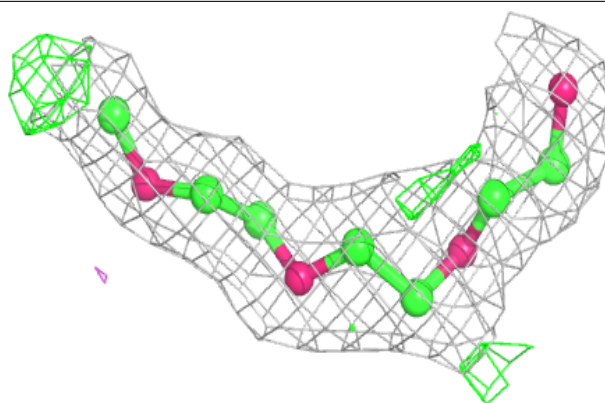
**Electron density around C8E D 402:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

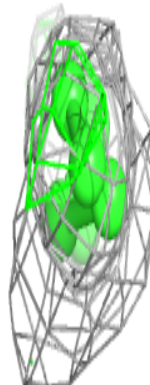
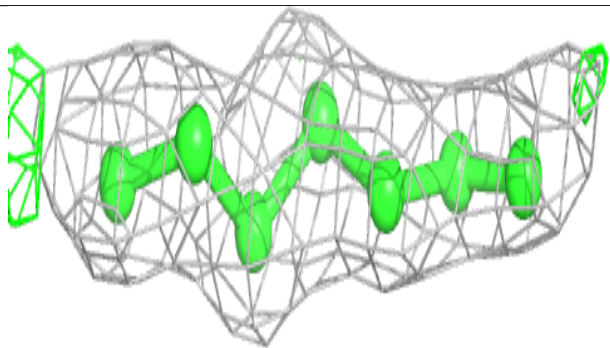
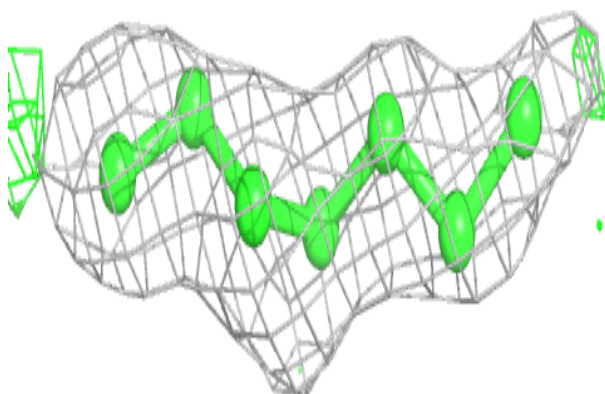


Electron density around C8E A 504:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

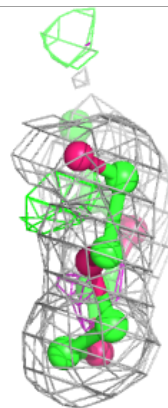
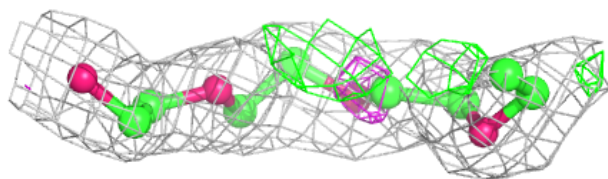
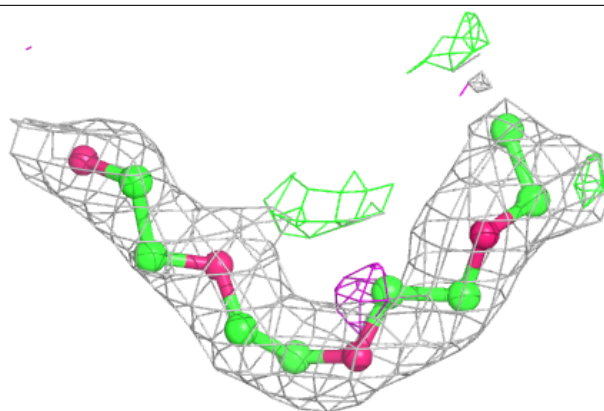
**Electron density around C8E E 402:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

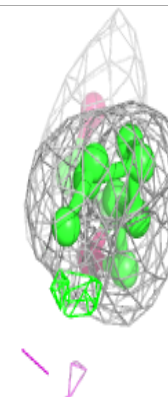
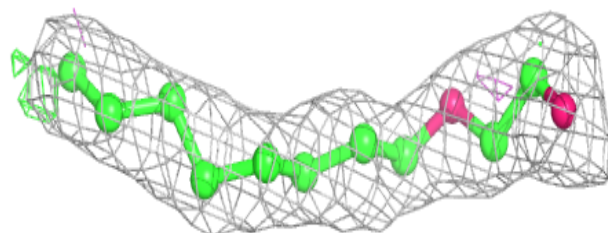
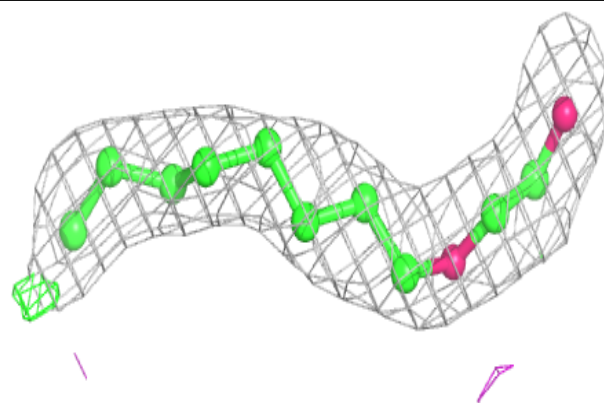


Electron density around C8E B 807:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

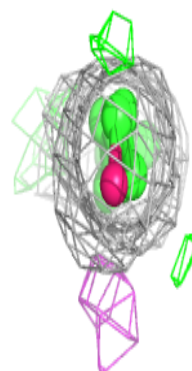
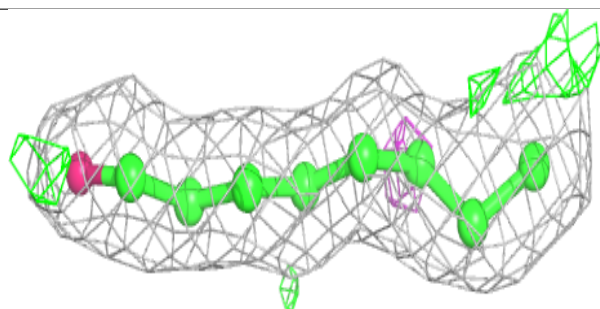
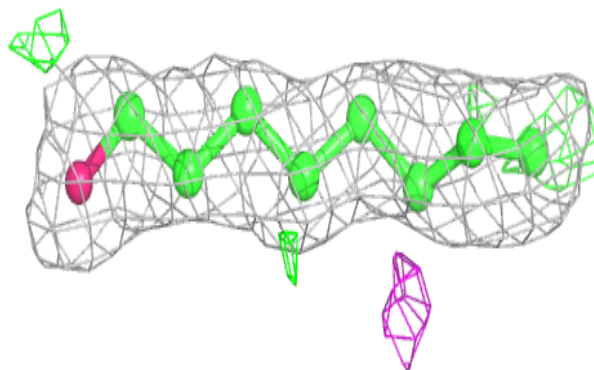
**Electron density around C8E D 403:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

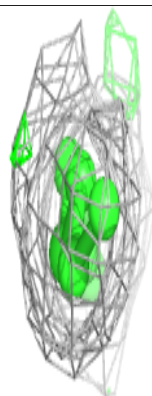
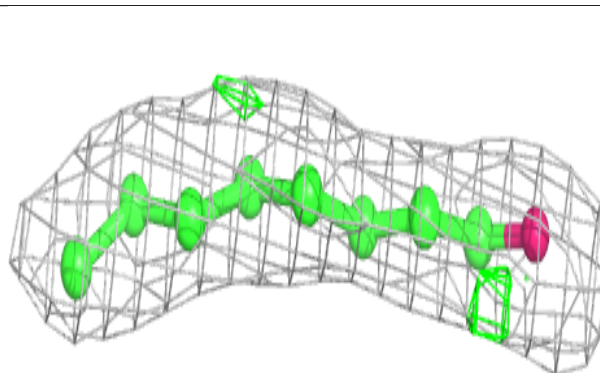
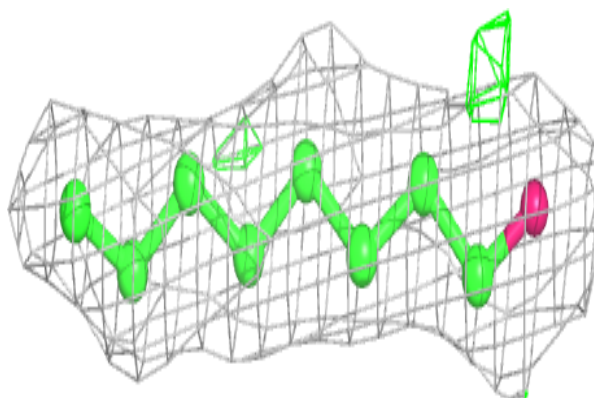


Electron density around C8E A 502:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

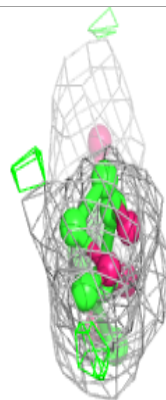
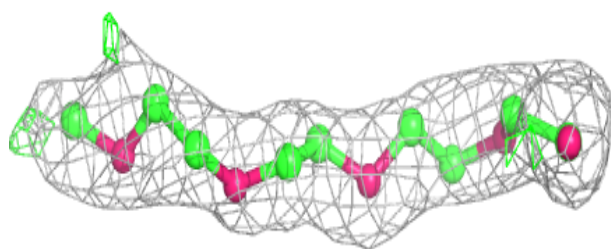
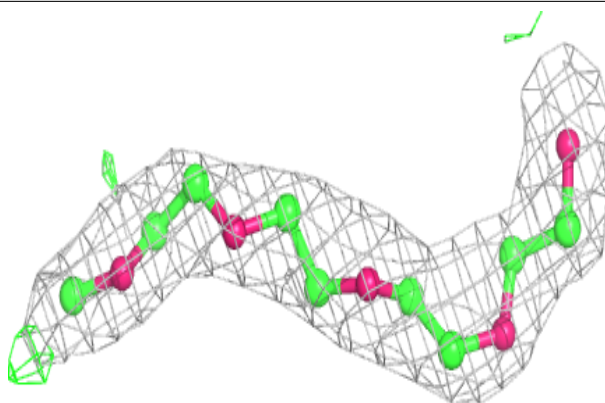
**Electron density around C8E E 401:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

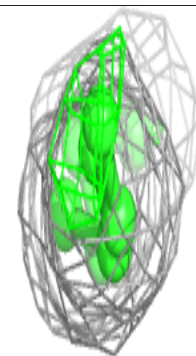
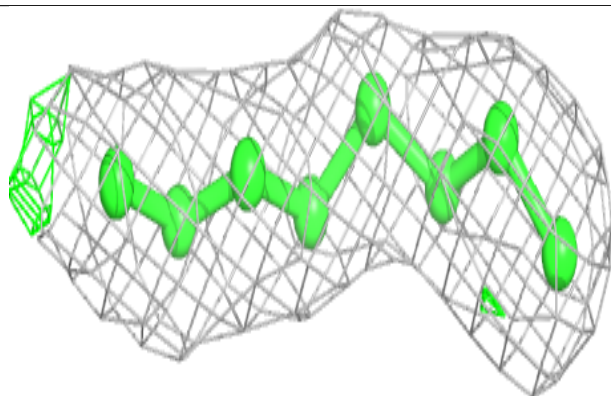
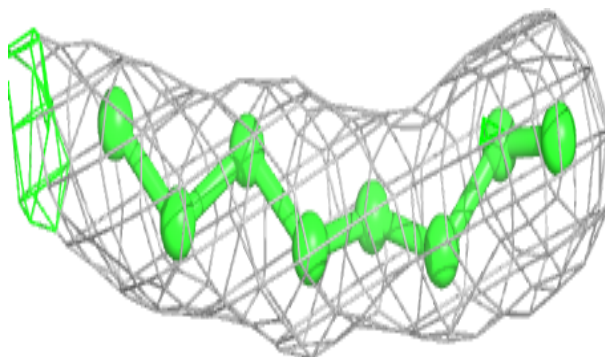


Electron density around C8E A 503:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

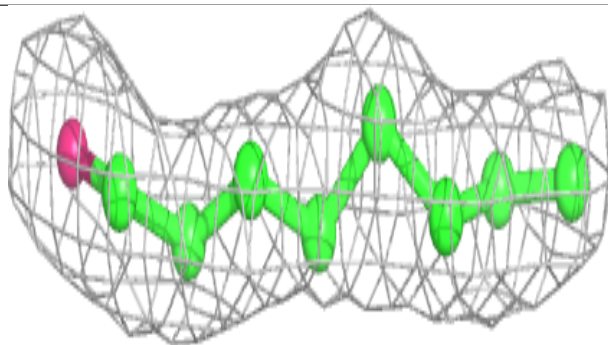
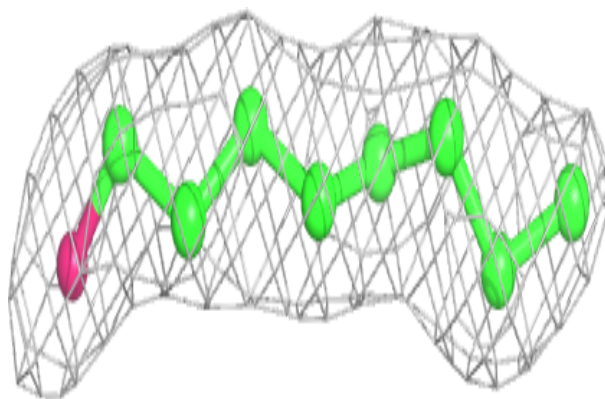
**Electron density around C8E B 805:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

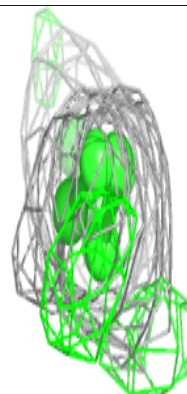
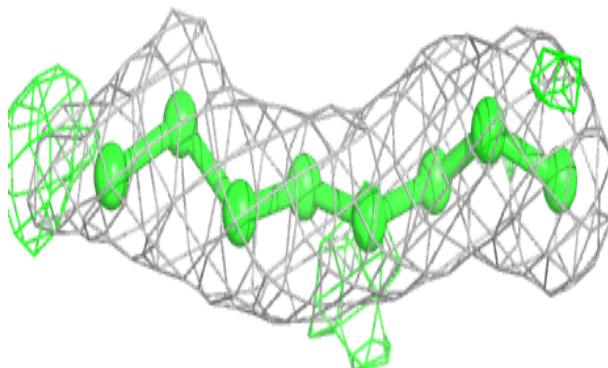
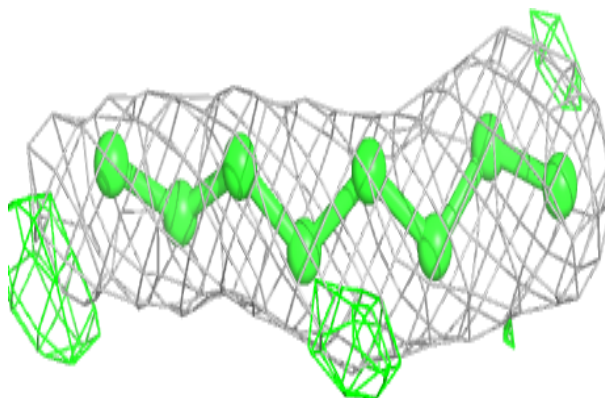


Electron density around C8E A 501:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

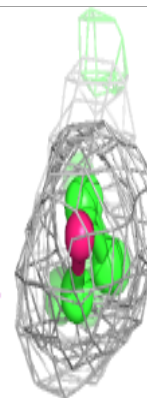
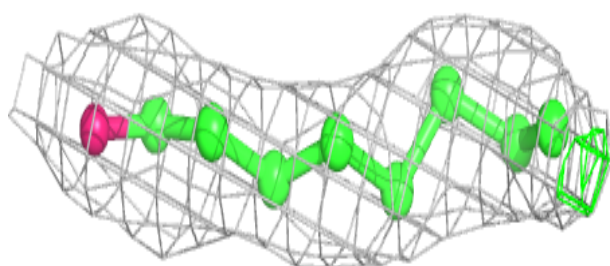
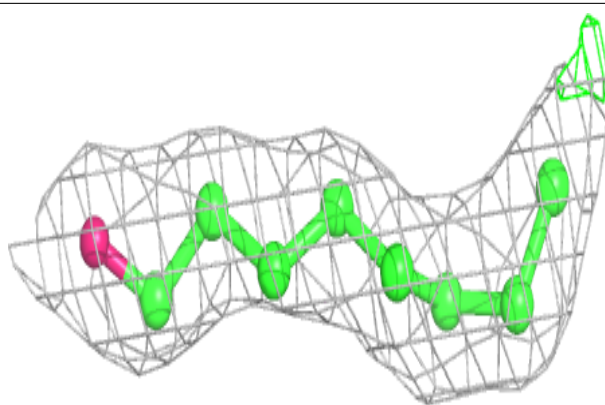
**Electron density around C8E F 401:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

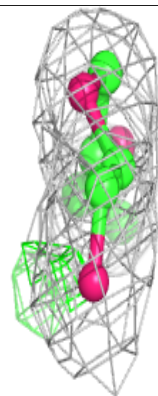
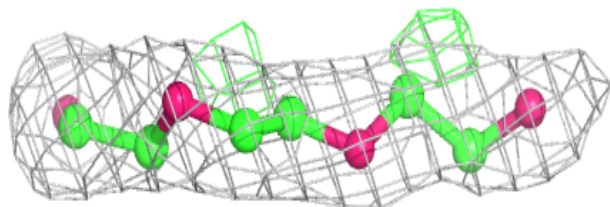
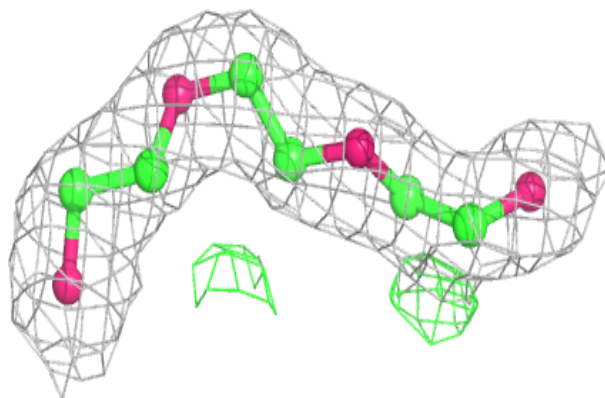


Electron density around C8E B 804:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

**Electron density around C8E E 404:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



6.5 Other polymers [i](#)

There are no such residues in this entry.